BLOCH ELECTRONS IN CROSSED ELECTRIC AND MAGNETIC FIELDS

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Presently used methods of treating the problem of an electron moving in a periodic potential, perturbed by the presence of crossed electric and magnetic fields, and their limitations, are discussed. The wave functions and the energy levels of such an electron are calculated by means of a modified perturbation theory, which has been previously successfully applied to the case of a magnetic field alone. A complete set of basis functions, in which to expand the wave functions, is introduced. These basis functions are taken to be products of the field-free wave functions and the harmonic oscillator functions associated with a free electron in crossed electric and magnetic fields. An application to the case of an ellipsoidal band is carried out, and the results are compared with those obtained from the usual effective mass formalism.

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A thesis submitted to
the Board of Graduate Studies
in partial fulfilment of the
requirements for the degree of
Master of Science

Department of Physics
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Montreal

August 1969

ACKNOWLEDGEMENTS

The author wishes to thank Dr. S. P. Morris for suggesting this thesis problem, and for laying all of the groundwork without which this thesis would not have been produced.

ABSTRACT

Presently used methods of treating the problem of an electron moving in a periodic potential, perturbed by the presence of crossed electric and magnetic fields, and their limitations, are discussed. The wave functions and the energy levels of such an electron are calculated by means of a modified perturbation theory, which has previously been successfully applied to the case of a magnetic field alone. A complete set of basis functions, in which to expand the wave functions, is introduced. These basis functions are taken to be products of the field-free wave functions and the harmonic oscillator functions for a free electron in crossed electric and magnetic fields. An application to the case of an ellipsoidal band is carried out, and the results are compared with those obtained from the usual effective mass formalism.

TABLE OF CONTENTS

CHAPTER 1

INTRODUCTION

In order to study experimentally the properties of a solid, external electric and magnetic fields are usually imposed. The effects of these external influences are then measured. Such measurements can yield a great deal of information concerning the band structure of the material under observation once they are related to the behaviour of the electrons in the solid. This relationship is obtained theoretically by adding the perturbing terms due to the external fields to the crystal Hamiltonian resulting in a many-particle Schrödinger equation. Because of the enormous difficulties of solving such an equation, it is usual to resort to approximation methods in order to proceed any further.

The question of how these external fields modify the band structure of a solid has proved to be a difficult one. The earliest investigations of magnetic states in crystals attempted to account for the diamagnetic supsceptibility of the conduction electrons in metals. This was first done by Landau(1) who treated the conduction electrons as free electrons in a magnetic field. The Hamiltonian used in the wave equation for this problem is in the form:

$$H = \frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2$$

Peierls(2) then considered the effect of the lattice potential on the eigenstates. He did this by attempting a solution as a linear combination of atomic orbitals. In the absence of external fields and in the limit of tight binding, an atomic orbital is an adequate local solution of the Schrödinger equation. However, under a shift through a lattice vector, the Hamiltonian preserves its form while the vector potential $\vec{A}$ changes in a manner which corresponds to a gauge transformation. Because of this, Peierls found it necessary to modify each shifted orbital by multiplying it by a phase factor so that it corresponds to a local solution in the new gauge. Using these phase factors, Peierls found that energy eigenvalues could be obtained as eigenvalues of an operator $E(\vec{P}/\hbar)$, the effective Hamiltonian, and where $\vec{P} = \vec{p} + \frac{e\vec{A}}{c}$ and $E(\vec{K})$ is the energy band function. The question of the generality of the result has persisted until the present time.

The weakness of Peierls' derivation comes from his use of atomic orbitals as basis functions. These are not orthonormal and are only approximately so in the limit of tight binding. Wannier(3) introduced a set of orthonormal functions $a_n(\vec{r}-\vec{R}_m)$ which span the space of Bloch functions from a single band. By using these it is possible to formulate a rigorous effective Hamiltonian for non-magnetic problems. Luttinger(4) removed the tight-binding approximation from the magnetic problem by using Wannier functions in place of atomic orbitals. However, the incorporation of Peierls' phase factor destroyed the orthonormal properties of these functions so that this formulation is still not exact, and the approximation is expected to worsen with increasing magnetic fields. Kohn(5) then attempted to find an effective Hamiltonian which would be valid for all fields. Such a function was obtained in the form of a power series $\sum_n f_n B^n$, where $\vec{B}$ is the magnetic field strength. In this expression the leading term is given by $E(\vec{P}/\hbar)$. Blount(6) and Roth(7) independently obtained simplified proofs of Kohn's results. These derivations are usually referred to as asymptotic expansion methods. However, the existence of an effective Hamiltonian is still not yet firmly established by these methods, since the expansions have not been shown to converge. This has led several authors(8-11) to arrive at an effective Hamiltonian by an alternate method, that of considering the translational properties of the Hamiltonian.

The asymptotic expansion methods yield an expression for H_{eff} with $E(\vec{P}/\hbar)$ as the leading term in a power series in B. The succeeding terms in the series become progressively more complicated and explicit formulae have been given only up to the quadratic term. For some problems, such as the case of a spinless electron near a non-degenerate band edge of a semiconductor having simple energy surfaces, it is sufficient to use just the leading term. This will result in an effective Schrödinger equation in which the free electron mass is replaced by an effective mass m*. Luttinger and Kohn(12) had previously arrived at this result for the case cited above by assuming that, at any instant of time, the wave function for the electron is a superposition of states from different bands. By introducing a suitable set of basis functions it is possible to expand the perturbed solution in terms of these functions. The generalization of this approach is referred to as the effective mass approximation(EMA), and has been widely used to explain a number of phenomena, including the one under consideration here, associated with the motion of an electron in a perturbed periodic potential. Not surprisingly, as will be seen, these results are severely limited. In particular the results are inapplicable if interband matrix elements are involved(13), nor are they easily extended to non-parabolic bands.

In an attempt to avoid these limitations, Morris(14) has started with a different set of basis functions. By avoiding functions which are infinitely extended in space such as plane wave or Bloch functions, he was able to use the results of standard perturbation theory to calculate the wave functions of an electron in a magnetic field. The harmonic oscillator functions are relatively localized, and moreover, occur naturally when the wave equation for a free electron in a magnetic field is solved. These are thus a logical choice to form part of the basis functions.

It is implicit that a successful theory should be able to handle simultaneous magnetic and electric fields. The present work is an attempt to extend the formalism to the case of crossed electric and magnetic fields. In the next chapter the development and results of the EMA are briefly reviewed with emphasis on those aspects related to the problem of crossed fields and the limitations of the method. In Chapter 3, the basis functions are introduced and discussed. Following this, a perturbation approach is taken to evaluate the expansion coefficients up to second order. The resulting wave functions are then confirmed to form an orthonormal set, and finally the results are applied to an ellipsoidal band and the connection with the EMA is shown.

CHAPTER 2

THE EFFECTIVE MASS APPROXIMATION

2.1 The EMA for Electrons in Crossed Fields

In dealing with problems related to the motion of electrons in semiconductors, where only states near an energy band maximum or minimum are involved, the usual approach is to use the EMA. There have been several derivations of an effective mass theorem; the one followed here is due to the work of Luttinger and Kohn(12), hereafter referred to as LK. In their original paper, two cases were treated in detail: 1) motion in the field of an impurity atom and 2) motion in a constant magnetic field.

The LK treatment is suitable for the crossed field configuration, and has been used by several authors for this purpose(15-19). We shall begin with Schrödinger's equation for an electron moving in a periodic potential perturbed by a constant magnetic field

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{2-1}$$

and a constant electric field

$$\vec{E} = -\vec{\nabla}\phi \tag{2-2}$$

perpendicular to $\vec{B}$.

$$\left\{ \frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 - e\phi(\vec{r}) + V(\vec{r}) \right\} \Psi = \varepsilon \Psi \tag{2-3}$$

where $\vec{p}$ is the momentum of the electron, e is the absolute value of the electron charge,

c is the velocity of light,

$V(\vec{r})$ is the periodic potential,

m is the mass of the free electron,

$\vec{A}$ is the vector potential,

$\phi(\vec{r})$ is the scalar potential.

It is convenient to introduce a special gauge, the Landau gauge, to handle the problem:

$$\vec{E} = (E,\ 0,\ 0) \tag{2-4}$$

$$\vec{A} = (-By,\ 0,\ 0) \tag{2-5}$$

In this special gauge, it can be shown from Appendix A that the Hamiltonian can be written in the form:

$$H = H_o - \omega_c y p_x + \tfrac{1}{2} m \omega_c^2 y^2 - e\phi(\vec{r})$$

$$H_o = \frac{p^2}{2m} + V(\vec{r})$$

$$\omega_c = \frac{eB}{mc} = \text{cyclotron frequency}$$

In the LK representation, we choose a complete orthonormal set of functions

$$\chi_{n\vec{k}} = \exp(i\vec{k}\cdot\vec{r})\, u_{no}(\vec{r}) \tag{2-6}$$

where $u_{no}(\vec{r})$ are Bloch functions at the bottom of the n^{th} band. In other words,

$$\Psi = \sum_{n'} \int_{\vec{k}' < B.Z.} A_{n'}(\vec{k}')\, \chi_{n'\vec{k}'}\, d^3\vec{k}'$$

which after substitution into (2-3) results in

$$\sum_{n'} \int \langle n\vec{k} | H_o + H' | n'\vec{k}' \rangle A_{n'}(\vec{k}')\, d^3\vec{k}' = \varepsilon A_n(\vec{k}) \tag{2-7}$$

where the notation $\langle n\vec{k}|H_o+H'|n'\vec{k}'\rangle$ means the matrix element with respect to $\chi_{n\vec{k}}$, and

$$H' = -\omega_c y p_x + \tfrac{1}{2} m\omega_c^2 y^2 + eEx$$

These are to be evaluated as follows:

$$\langle n\vec{k}|H_o|n'\vec{k}'\rangle = \int \exp(-i\vec{k}\cdot\vec{r})\, u_{no}^*\, H_o \exp(i\vec{k}'\cdot\vec{r})\, u_{n'o}(\vec{r})\, d^3\vec{r}$$

$$= \int \exp(-i\vec{k}\cdot\vec{r})\, u_{no}^* \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right) \exp(-i\vec{k}'\cdot\vec{r})\, u_{n'o}(\vec{r})\, d^3\vec{r}$$

and with the operator equivalence

$$\vec{p} \equiv -i\hbar\vec{\nabla}$$

$$\vec{p}\,\chi_{n'\vec{k}'} = \exp(i\vec{k}'\cdot\vec{r})(\vec{p} + \hbar\vec{k}')\, u_{n'o}(\vec{r})$$

$$\langle n\vec{k}|H_o|n'\vec{k}'\rangle = \int \exp[i(\vec{k}'-\vec{k})\cdot\vec{r}]\, u_{no}^* \left[\frac{p^2}{2m} + \frac{\hbar^2 k'^2}{2m} + \frac{\hbar\vec{k}'\cdot\vec{p}}{m} + V(\vec{r})\right] u_{n'o}\, d^3\vec{r}$$

$$= \int \exp[i(\vec{k}'-\vec{k})\cdot\vec{r}]\, u_{no}^* \left[H_o + \frac{\hbar\vec{k}'\cdot\vec{p}}{m} + \frac{\hbar^2 k'^2}{2m}\right] u_{n'o}\, d^3\vec{r}$$

$$= \int \exp[i(\vec{k}'-\vec{k})\cdot\vec{r}]\, u_{no}^* \left[\varepsilon_{n'o} + \frac{\hbar\vec{k}'\cdot\vec{p}}{m} + \frac{\hbar^2 k'^2}{2m}\right] u_{n'o}\, d^3\vec{r}$$

where $\quad H_o u_{n'o} = \varepsilon_{n'o} u_{n'o}$

$$\langle n\vec{k}|H_o|n'\vec{k}'\rangle = \sum_{\vec{R}_m} \exp[i(\vec{k}'-\vec{k})\cdot\vec{R}_m] \int_{\substack{unit\\cell}} u_{no}^* \left(\varepsilon_{n'o} + \frac{\hbar\vec{k}'\cdot\vec{p}}{m} + \frac{\hbar^2 k'^2}{2m}\right) u_{n'o}\, d^3\vec{r}'$$

$$= N\,\delta(\vec{k}-\vec{k}') \int_{\substack{unit\\cell}} u_{no}^* \left(\varepsilon_{n'o} + \frac{\hbar\vec{k}'\cdot\vec{p}}{m} + \frac{\hbar^2 k'^2}{2m}\right) u_{n'o}\, d^3\vec{r}'$$

$$= \delta(\vec{k}-\vec{k}') \left[\left(\varepsilon_{n'o} + \frac{\hbar^2 k'^2}{2m}\right)\delta_{nn'} + \frac{\hbar k_\alpha p^{(\alpha)}_{nn'}}{m}\right] \qquad (2\text{-}8)$$

In the above we have used the relationship $\vec{r} = \vec{r}' + \vec{R}_n$, where $\vec{R}_n$ is a translation vector joining the point $\vec{r}$ to a point $\vec{r}'$ which is confined to a fundamental unit cell. In this case, it can be shown that

$$\sum_{\vec{R}_n} \exp i(\vec{k}' - \vec{k}) \cdot \vec{R}_n = N\delta(\vec{k} - \vec{k}' + \vec{K}_m)$$

where $\vec{K}_m$ is a vector of the reciprocal lattice. However, since $\vec{k}$ and $\vec{k}'$ are both in the first Brillouin zone, $\vec{k} - \vec{k}' = \vec{K}_m$ is only possible if $m = 0$. Thus

$$\sum_{\vec{R}_n} \exp i(\vec{k}' - \vec{k}) \cdot \vec{R}_n = N\delta(\vec{k} - \vec{k}') \qquad (2\text{-}9)$$

Also in equation (2-8), a summation over $\alpha = x, y, z$ is implied. The quantities $p^{(\alpha)}_{nn'}$ are just the momentum matrix elements at the bottom of the band, having the properties

$$p^{(\alpha)}_{nn'} = -p^{(\alpha)}_{n'n} \quad , \quad p^{(\alpha)}_{nn} = 0 \qquad (2\text{-}10)$$

We have also used the orthogonality of the Bloch functions.

Proceeding in a similar manner for H',

$$\langle n\vec{k}|H'|n'\vec{k}'\rangle$$

$$= -\omega_c \langle n\vec{k}|yp_x|n'\vec{k}'\rangle + \frac{m\omega_c^2}{2}\langle n\vec{k}|y^2|n'\vec{k}'\rangle - \langle n\vec{k}|e\phi|n'\vec{k}'\rangle$$

$$= -\omega_c \int \exp i(\vec{k}' - \vec{k}) \cdot \vec{r}\; u^*_{n0}\, y(\hbar k_x - i\hbar\nabla_x) u_{n'0}\, d^3\vec{r}$$

$$+ \tfrac{1}{2} m\omega_c^2 \int y^2 \exp i(\vec{k} - \vec{k}') \cdot \vec{r}\; u^*_{n0} u_{n'0}\, d^3\vec{r}$$

$$- \langle n\vec{k}|e\phi|n'\vec{k}'\rangle$$

Using an argument identical to the one used in deriving equation (2-8), the Hamiltonian due to the perturbing terms can now be written in the form:

$$\langle n\vec{k}|H'|n'\vec{k}'\rangle$$

$$= i\omega_c \frac{\partial}{\partial k_y'}\left[(\hbar k_x \delta_{nn'} + p_{nn'}^{(x)})\,\delta(\vec{k}-\vec{k}')\right] - \frac{1}{2} m\omega_c^2 \frac{\partial^2 \delta(\vec{k}-\vec{k}')}{\partial k_y'^2}\,\delta_{nn'} - \langle n\vec{k}|e\phi|n'\vec{k}'\rangle$$

In the LK representation, then

$$\langle n\vec{k}|H|n'\vec{k}'\rangle$$

$$= \Big[(\varepsilon_{n'o} + \frac{\hbar^2 k'^2}{2m})\,\delta(\vec{k}-\vec{k}') + i\omega_c \hbar k_x \frac{\partial \delta(\vec{k}-\vec{k}')}{\partial k_y'} - \frac{1}{2} m\omega_c^2 \frac{\partial^2 \delta(\vec{k}-\vec{k}')}{\partial k_y'^2}\Big]\delta_{nn'} + \frac{h k_\alpha}{m} p_{nn'}^{(\alpha)}\,\delta(\vec{k}-\vec{k}') + i\omega_c p_{nn'}^{(x)} \frac{\partial \delta(\vec{k}-\vec{k}')}{\partial k_y'} - \langle n\vec{k}|e\phi|n'\vec{k}'\rangle \tag{2-11}$$

The aim of the EMA is to eliminate all non-diagonal elements by applying a diagonalization procedure to the Hamiltonian. The matrix element $\langle n\vec{k}|e\phi|n'\vec{k}'\rangle$ can generally be expressed as a Fourier series. At this point, it is usual to stipulate that the potential be a gentle potential, the word gentle meaning that the potential does not change appreciably over a unit cell, so that only the first term of the series need be kept. If this is the case, the matrix $\langle n\vec{k}|e\phi|n'\vec{k}'\rangle$ can generally be treated as diagonal.

$$\langle n\vec{k}|e\phi|n'\vec{k}'\rangle = e\,\phi(\vec{k}-\vec{k}')\,\delta_{n'n}$$

$$\phi(\vec{k}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}}\int \phi(\vec{r})\exp(-i\vec{k}\cdot\vec{r})\,d^3\vec{r}$$

We now have all the information needed to write down the Hamiltonian in a succinct form.

$$H = H_B^{(D)} + H_E^{(D)} + H_M^{(D)} + H_B^{(ND)} + H_M^{(ND)} \tag{2-12}$$

$$\langle n\vec{k}|H_B^{(D)}|n'\vec{k}'\rangle = \left(\mathcal{E}_{n'0} + \frac{\hbar^2 k'^2}{2m}\right)\delta_{nn'}\,\delta(\vec{k}-\vec{k}') \tag{2-13}$$

$$\langle n\vec{k}|H_M^{(D)}|n'\vec{k}'\rangle = \left\{ i\omega_c \frac{\partial\delta(\vec{k}-\vec{k}')}{\partial k_y'}\hbar k_x - \frac{m\omega_c^2}{2}\frac{\partial^2\delta(\vec{k}-\vec{k}')}{\partial k_y'^2}\right\}\delta_{nn'} \tag{2-14}$$

$$\langle n\vec{k}|H_E^{(D)}|n'\vec{k}'\rangle = -e\,\phi(\vec{k}-\vec{k}')\,\delta_{nn'} \tag{2-15}$$

$$\langle n\vec{k}|H_B^{(ND)}|n'\vec{k}'\rangle = \frac{1}{m}\hbar k_\alpha p_{nn'}^{(\alpha)}\,\delta(\vec{k}-\vec{k}') \tag{2-16}$$

$$\langle n\vec{k}|H_M^{(ND)}|n'\vec{k}'\rangle = +i\omega_c p_{nn'}^{(x)}\frac{\partial\delta(\vec{k}-\vec{k}')}{\partial k_y'} \tag{2-17}$$

Here, the subscripts B, M, E imply Bloch, magnetic and electric terms; the superscripts (D), (ND) imply, in turn, diagonal and non-diagonal terms. In order to arrive at an effective Hamiltonian, it is necessary that all non-diagonal terms be reduced to the lowest order. This is done by means of a canonical transformation. Applying an operator e^S to the Hamiltonian of equation (2-12), we get

$$\bar{H} = \exp(-S)H\exp(S)$$

$$\bar{H} = H_B^{(D)} + H_E^{(D)} + H_M^{(D)} + H_B^{(ND)} + H_M^{(ND)} + [H_B^{(D)}, S] + [H_M^{(D)}, S]$$
$$+ [H_E^{(D)}, S] + [H_M^{(ND)}, S] + [H_B^{(ND)}, S]$$
$$+ \frac{1}{2}[[H_B^{(D)}, S], S] + \text{---} \qquad (2\text{-}18)$$

All higher order terms may be safely neglected if S is sufficiently small. In that case, the only further stipulation necessary to remove all non-diagonal terms is that

$$[H_B^{(D)}, S] + H^{(ND)} = 0 \qquad (2\text{-}19)$$

$[H_M^{(D)}, S]$, $[H_E^{(D)}, S]$ is negligible

From these conditions, it is possible to determine the explicit form of S

$$\langle n\vec{k}|S|n'\vec{k}'\rangle = -\frac{\frac{1}{m}\left[\hbar k_\alpha p_{nn'}^{(\alpha)}\delta(\vec{k}-\vec{k}') + im\omega_c p_{nn'}^{(x)}\frac{\partial\delta(\vec{k}-\vec{k}')}{\partial k_y'}\right]}{\hbar\omega_{nn'}}$$
$$= 0 \qquad n = n' \qquad (2\text{-}20)$$

$$\hbar\omega_{nn'} = \varepsilon_{no} - \varepsilon_{n'o} \qquad (2\text{-}21)$$

Inserting (2-20) into (2-18) yields the effective Hamiltonian in the form

$$H^* = H_B^{(D)*} + H_M^{(D)*} + H_E^{(D)*} \qquad (2\text{-}22)$$

where

$$\langle n\vec{k}|H_B^{(D)*}|n'\vec{k}'\rangle = \left[\varepsilon_{n'o} + \frac{1}{2}\left(\frac{\partial^2\varepsilon_{n'}(\vec{k})}{\partial k_\alpha\partial k_\beta}\right)_o k_\alpha k_\beta\right]\delta_{nn'}\delta(\vec{k}-\vec{k}') \qquad (2\text{-}23)$$

$$\langle n\vec{k}|H_M^{(D)*}|n'\vec{k}'\rangle = [m\omega_c \hbar k_\alpha \left(\frac{\partial^2\varepsilon_n(\vec{k})}{\partial k_\alpha\partial k_x}\right)_o \frac{1}{i}\frac{\partial\delta(\vec{k}-\vec{k}')}{\partial k_y'}$$

$$+ \frac{1}{2i}\left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_x \partial k_y}\right)_0 \delta(\vec{k}-\vec{k}')\Big\} - \frac{1}{2} m\omega_c^2 \frac{\partial^2 \delta(\vec{k}-\vec{k}')}{\partial k_y'^2}\Big]\delta_{nn'} \qquad (2\text{-}24)$$

The electric term remains unchanged. $\mathcal{E}_n(\vec{k})$ is the energy band function. Details are available in reference (12).

The effect of the canonical transformation on the original wave function is to produce a new wave function $B_n(\vec{k})$ defined by $A(\vec{k}) = \exp(S)B(\vec{k})$

$$A_n(\vec{k}) = \sum_n \int \langle n\vec{k}| e^S | n'\vec{k}'\rangle B_{n'}(\vec{k}')\, d^3\vec{k}' \qquad (2\text{-}25)$$

In this representation Schrödinger's equation becomes

$$(H_B^{(D)*} + H_M^{(D)*} + H_E^{(D)*})\, B_n(\vec{k}) = \varepsilon B_n(\vec{k}) \qquad (2\text{-}26)$$

$$\mathcal{E}_n(\vec{k}) B_n(\vec{k}) + m\omega_c\hbar \Big\{ k_\alpha \left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_\alpha \partial k_x}\right)_0 i \frac{\partial B_n(\vec{k})}{\partial k_y}\Big\}$$

$$- \frac{1}{2} m\omega_c^2 \left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_x^2}\right)_0 i^2 \frac{\partial^2 B_n(\vec{k})}{\partial k_y^2} + \frac{m\omega_c\hbar}{2i}\left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_x \partial k_y}\right)_0 B_n(\vec{k})$$

$$- e\phi\, B_n(\vec{k}) = \varepsilon B_n(\vec{k})$$

To obtain the wave function in co-ordinate space, we need only define

$$F_n(\vec{r}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int_{\vec{k} < B.Z.} [\exp(i\vec{k}\cdot\vec{r})]\, B_n(\vec{k})\, d^3\vec{k}$$

from which the equation becomes

$$\left[\mathcal{E}_n(-i\vec{\nabla} + \frac{e\vec{A}}{c}) - e\phi(\vec{r})\right] F_n(\vec{r}) = \varepsilon F_n(\vec{r}) \qquad (2\text{-}27)$$

Thus, we see that in the presence of a crossed field, the function $F_n(\vec{r})$ satisfies the differential equation which is obtained by using the expansion of $\mathcal{E}_n(\vec{k})$ to quadratic terms as the Hamiltonian, and replacing $\vec{k}$ by the operator $(-i\hbar\vec{\nabla} + \frac{e\vec{A}}{c})$.

2.2 Applicability of the EMA

As its name implies, the EMA is an approximate theory. In this section, the conditions of its applicability will be discussed.

In developing the result, three assumptions were made:

1) The potential $\phi(\vec{r})$ must be given by a diagonal matrix in the LK representation.

2) The terms $[H_M^{(0)}, S]$ and $[H_E^{(0)}, S]$ in (2-15) must be small in comparison with the terms in the effective Hamiltonian.

3) In addition to these requirements, it was further assumed that the matrix $S \ll 1$. From (2-20), this leads to the condition

$$\left.\begin{aligned} -\frac{p_{nn'}^{(y)}}{m\omega_{nn'}} k_y \ll 1 \\ -\frac{p_{nn'}^{(z)}}{m\omega_{nn'}} k_z \ll 1 \end{aligned}\right\} \qquad (2\text{-}28)$$

$$-\,p_{nn'}^{(x)}\left(k_x + i m\omega_c \frac{\partial}{\partial k_y}\right) \ll 1 \qquad (2\text{-}29)$$

where the values of k_y, k_z and $(k_x + i m\omega_c \frac{\partial}{\partial k_y})$ are to be evaluated in the states which are given by the solutions of the effective mass Hamiltonian. Thus, to find whether the EMA is valid, we have to find whether its solution $F_n(\vec{r})$ can be written in the form of a Fourier integral where the integration is only over these values of $\vec{k}$ that satisfy these conditions.

If the formalism is now applied to the simple case of a non-degenerate spherical band

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$$

where m* denotes the effective mass, then the effective mass equation can be put in the form

$$\left[\frac{1}{2m^*}\left(-i\hbar\vec{\nabla} + \frac{e\vec{A}}{c}\right)^2 + e\vec{E}\cdot\vec{r} \right] F(\vec{r}) = \varepsilon F(\vec{r}) \tag{2-30}$$

The solution of this type of equation is given in Appendix A, and expressed in terms of the harmonic oscillator functions of argument

$$\frac{x + \lambda^2(k_y + mcE/\hbar B)}{\lambda}$$

These functions contain Hermite polynomials, and from the properties of these latter functions(20) we know that if $H_N(\xi)$ represents the Hermite polynomial, $H_N(\xi)$ approaches zero very fast as ξ moves past the classical turning points, i.e., when $\xi \gg |2N+1|^{\frac{1}{2}}$

The following analysis can then be made(18) in this case:

$$-(2N+1)^{\frac{1}{2}} \leq \frac{x + \lambda^2(k_y + \frac{mcE}{\hbar B})}{\lambda} \leq (2N+1)^{\frac{1}{2}}$$

The limiting value of k_y is then given by

$$k_y = -\frac{(2N+1)^{\frac{1}{2}}}{\lambda} - \frac{mcE}{\hbar B}$$

It has already been shown that the EMA procedure requires

$$-k_y a \ll 1 , \qquad a = \frac{p^{(y)}_{nn'}}{m\,\omega_{nn'}}$$

and this leads to the requirements

$$\frac{(2N+1)^{\frac{1}{2}}a}{\lambda} << 1$$

$$\frac{m^{*}cEa}{\hbar B} << 1$$

This imposes two further restrictions on the EMA. This was first pointed out in reference (18), and would account for the discrepancy between the results predicted by Aronov(15) and those obtained experimentally by Reine et al(21). In his paper, Aronov employed the EMA to calculate the optical interband absorption coefficient in crossed electric and magnetic fields. It was found that the location of the absorption maximum is a function of the field E, and that the energy gap in semiconductors decreases proportionally as $(cE/B)^2$. This was verified with a sample of germanium, but only for low values of the ratio (cE/B). For high values of (cE/B), the only effect of the magnetic field appeared to be that of reducing the absorption to below its value for $\vec{B}=0$.

2.3 The Two-Band Model

In this section, we shall look briefly at the two-band model which attempted to further the range of use of the EMA. It was proposed by Zawadzki and Lax(22) that the problem be treated as one of two coupled bands in order to take into account the non-parabolicity of the bands of actual semiconductors. They derived a simplified two-band equation which neglected the symmetry character of the bands involved (whether they were s- or p-like, etc). However it was subsequently shown by Weiler et al (23) that the resulting equation for the conduction band, which has an s-like characteristic, is unaffected by this symmetry. In the LK representation then, analogous to equation (2-30), the set of two equations for the envelope functions $F_n(\vec{r})$ for two coupled non-degenerate and spherical bands is written as:

$$\sum_{n'=1,2}\left\{\left[\frac{1}{2m^*}P^2 + e\vec{E}\cdot\vec{r} + \varepsilon_n - \varepsilon\right]\delta_{n'n} + \vec{P}\cdot\vec{\pi}_{n'n}\right\}F_{n'}(\vec{r}) = 0 \quad (2\text{-}31)$$

where $\vec{\pi}_{n'n} = (1/m)\langle u_{n'o}|\vec{p}|u_{no}\rangle$

Equation (2-31) can be reduced to a single equation, whose solution is not trivial but has been obtained(24). However, it is possible to make some qualitative remarks without actually solving this equation. These are summarized below:

(1) $\omega_c^2 \gg 2e^2E^2/m^*(\varepsilon_{10}-\varepsilon_{20})$, i.e., the electric term is negligible in comparison with the magnetic term. The equation then has bound harmonic oscillator solutions. If, in addition, only states with low quantum numbers are considered, the equation becomes the one-band effective mass equation in crossed fields, and the eigenvalues cross over to those obtained by Aronov.

(2) $\omega_c^2 \ll 2e^2E^2/m^*(\varepsilon_{10}-\varepsilon_{20})$, i.e., the electric field term is predominant. Under this condition, the

spectrum of eigenvalues is essentially continuous.

The two-band model outlined here has had a degree of success in explaining some experimentally observed phenomena. In the presence of a strong magnetic field or a crossed electric and magnetic field, the optical absorption near the absorption edge is observed to exhibit oscillations. In the crossed field configuration, it is further observed that, as the electric field is increased, there is a transition from the oscillatory magnetoabsorption to the Franz-Keldysh effect(25,26), that being the absorption of photons of energy less than the interband gap energy. The one-band EMA fails to predict this kind of behaviour, since, even for very weak magnetic fields. the bound oscillatory solutions are obtained.

2.4 Alternative Approach to the Problem

Because of the limitations of the one-band EMA, a different approach to the problem seemed to be called for. It was pointed out by Lax(27) that, in order to obtain the proper kind of solutions for the problem for high values of the ratio (cE/B), then, purely from classical considerations, it would be necessary to start with a non-parabolic equation of the relativistic type. This approach had already been taken by Wannier(8,9) who had replaced the original Schrödinger wave equation by another partial differential equation of higher dimensionality whose solutions and eigenvalues bear a definite relation to the solutions and eigenvalues of the original equation. Praddaude(10) used similar arguments to arrive at a different equation. In this section, we shall follow the methods of the latter since they have the advantage of corroborating the results of the previous section.

The basic idea underlying the approach is that externally applied fields must have a special relationship to the energy bands of a Bloch particle. Since the energy bands arise from the translational symmetry of the crystalline field, this symmetry should not be physically altered by the presence of the applied field. In the simplest case of an electron in a periodic potential, a convenient way to solve for the wave functions is to find three translational operators that commute with each other and with the Hamiltonian. The effect of these translational operators is to separate that part of the solution which has the lattice periodicity from the part which does not. The resulting wave functions are, of course, the well-known Bloch functions(e.g. 28).

$$\psi_B(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})\, u_{n\vec{k}}(\vec{r}) \tag{2-32}$$

$$u_{n\vec{k}}(\vec{r}+\vec{R}_m) = u_{n\vec{k}}(\vec{r})$$

However, when constant electric and magnetic fields are applied, the above procedure is no longer valid. The solution need not necessarily contain a part which has the periodicity of the lattice. It will be shown that by considering the effect of lattice translations on the Hamiltonian, the procedure will lead naturally to a "Bloch" function $b(\vec{r},\vec{k})$, whose eigenvalues correspond to the ones in the original problem.

The starting point is the familiar Schrödinger equation

$$\left\{ \frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 + e\vec{E}\cdot\vec{r} + V(\vec{r}) - \varepsilon \right\} \Psi(\vec{r}) = 0 \qquad (2\text{-}3)$$

Consider the effect of a lattice translation on (2-3). Changing the variable $\vec{r}$ to $\vec{r}+\vec{R}_n$ produces the equation

$$\left\{ \frac{1}{2m}\left(\vec{p} + \frac{e}{2c}\vec{B}\times(\vec{r}+\vec{R}_n)\right)^2 + e\vec{E}\cdot(\vec{r}+\vec{R}_n) + V(\vec{r}) \right\} \Psi(\vec{r}+\vec{R}_n)$$

$$= \varepsilon\,\Psi(\vec{r}+\vec{R}_n) \qquad (2\text{-}33)$$

Let us consider the functions

$$\exp\left[-i\vec{k}\cdot(\vec{r}+\vec{R}_n)\right]\Psi(\vec{r}+\vec{R}_n) \qquad (2\text{-}34)$$

They can be shown to satisfy the equation

$$\left\{ \frac{1}{2m}\left(\vec{p} + \hbar\vec{k} + \frac{e}{2c}\vec{B}\times i\hbar\vec{\nabla}_{\vec{k}}\right)^2 + e\vec{E}\cdot i\hbar\vec{\nabla}_{\vec{k}} + V(\vec{r}) - \varepsilon \right\}$$

$$\times \exp -i\vec{k}\cdot(\vec{r}+\vec{R}_n)\,\Psi(\vec{r}+\vec{R}_n) = 0 \qquad (2\text{-}35)$$

This would seem to imply that the set of functions (2-34) are particular solutions of equation (2-35). Then, we can claim that the most general periodic solutions of

(2-35) can be formed as a linear combination of this set of functions. In other words, the functions

$$b(\vec{r},\vec{k}) = \left(\frac{1}{2\pi}\right)^{3/2} \sum_{R_n} \exp -i\vec{k}\cdot(\vec{r}+\vec{R}_n)\,\Psi(\vec{r}+\vec{R}_n) \tag{2-36}$$

must satisfy the equation

$$\left\{ \frac{1}{2m}\left(\vec{p}+\hbar\vec{k}+\frac{e}{2c}\,(\vec{B}\times i\hbar\vec{\nabla}_k)\right)^2 + V(\vec{r}) + e\vec{E}\cdot i\hbar\vec{\nabla}_k - \mathcal{E}\right\} b(\vec{r},\vec{k}) = 0 \tag{2-37}$$

with the requirements that $b(\vec{r},\vec{k})$ must be finite, continuous and have the lattice periodicity. It should be noted that these functions have in no way been rigourously derived; rather an intuitive guess has been made and the only criterion for their existence is the quality of the results obtainable from them.

To transform back to a co-ordinate representation, the function (2-36) is written as

$$b(\vec{r},\vec{k}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int \exp(-i\vec{k}\cdot\vec{\rho})\,\Psi(\vec{\rho})\,F(\vec{\rho}-\vec{r})\,d^3\vec{\rho} \tag{2-38}$$

where $F(\vec{\rho}-\vec{r})$ is a delta function defined by

$$F(\vec{\rho}-\vec{r}) = \sum_{R_n} \delta(\vec{\rho}-\vec{r}-\vec{R}_n)$$

Equation (2-38) shows that $b(\vec{r},\vec{k})$ is the Fourier transform of a function $B(\vec{r},\vec{r}')$ where

$$\begin{aligned} B(\vec{r},\vec{r}') &\equiv \Psi(\vec{r}')\,F(\vec{r}'-\vec{r}) \\ &= \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int \exp(i\vec{k}\cdot\vec{r}')\,b(\vec{r},\vec{k})\,d^3\vec{k} \end{aligned}$$

Finally by taking the Fourier transform of (2-37),

$$\left[\frac{1}{2m}\left(\vec{p} - i\hbar\vec{\nabla}_\rho - \frac{e}{2c}\vec{B}\times\vec{\rho}\right)^2 + V(\vec{r}) - e\vec{E}\cdot\vec{\rho} - \varepsilon\right]$$

$$\times\ B(\vec{r},\vec{\rho}) = 0 \qquad (2\text{-}40)$$

The above equation can now be expanded in terms of a convenient set of periodic functions in $\vec{r}$. This procedure will yield an effective mass equation for the modulation functions $\Psi(\vec{\rho})$, which play the role of expansion coefficients.

If the above equation is now applied to the case of two parabolic and non-degenerate bands, it is found that the nature of the solutions will depend on the ratio E/B. Below a certain critical value of the magnetic field, the character of the solutions will change from discrete to continuous, thus confirming the results in the previous section.

An analogy between the two-band model and classical relativistic motion of an electron in crossed fields(29) can be drawn. The energy $2m_oc^2$ is replaced by $\varepsilon_g = \varepsilon_{10} - \varepsilon_{20}$, the free-electron mass m_o is replaced by m^*. For cE/B greater than $(\varepsilon_g/2m^*)^{\frac{1}{2}}$, the problem can be transformed by a suitable Lorentz transformation into that of an electric field alone. In this case, the quantum mechanical solutions are continuous. On the other hand, for cE/B smaller than $(\varepsilon_g/2m^*)^{\frac{1}{2}}$, the problem can be transformed to one of motion in a magnetic field alone with bound and quantized solutions. This type of reasoning was successfully applied by Rajagopal(30) who calculated the longitudinal dielectric constant of a Bloch electron gas in crossed fields.

Thus, we have examined the problem of a Bloch electron in crossed electric and magnetic fields from various points of view. We note that, so far, there has not been developed an explicit procedure for determining the solutions and eigenvalues of the Schrödinger equation corresponding to the problem. The next chapter will be an attempt to meet this need.

CHAPTER 3

PERTURBATION APPROACH

3.1 The Basis Functions

As already mentioned, an attempt to obtain an approximate solution of equation (2-3) will be made by treating the external crossed fields as a perturbation and making use of the appropriate theory.

$$\left[\frac{1}{2m}\left(\vec{p}+\frac{e\vec{A}}{c}\right)^2 + V(\vec{r}) + e\vec{E}\cdot\vec{r}\right]\Psi = E\Psi \qquad (2\text{-}3)$$

In the following, the magnetic field $\vec{B}$ will be assumed to act along the z-direction, and the electric field $\vec{E}$ will be assumed to act parallel to the x-axis, as before.

In order to proceed further, it is necessary to choose some complete set of functions in which to expand the state functions Ψ. This basis set is chosen as follows:

$$\psi^N_{n\vec{k}_\perp}(\vec{r}) = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left(\frac{ieBxy}{2c\hbar}\right) \exp(i\vec{k}_\perp\cdot\vec{r})\, f^N_{k_y}(x)\, u_{no}(\vec{r}) \qquad (3\text{-}1)$$

where $\vec{k}_\perp = (0, k_y, k_z)$ and is restricted to the first Brillouin zone

$u_{no}(\vec{r})$ = periodic part of the Bloch function $\phi_{nk}(\vec{r})$

$$\phi_{nk}(\vec{r}) = \frac{1}{\sqrt{V}}\, u_{nk}(\vec{r}) \exp(i\vec{k}\cdot\vec{r}) \qquad (3\text{-}2)$$

with $\vec{k} = 0$

$$f^N_{k_y}(x) \equiv f^N_{k_y}\left(\frac{x + \lambda^2 k_y + \lambda^2 mcE/\hbar B}{\lambda}\right) \qquad (3\text{-}3)$$

The functions (3-3) are the harmonic oscillator functions centred about the point $x = -(\lambda^2 k_y + \lambda^2 mcE/\hbar B)$ for the energy levels specified by the integer N. The quantity $\lambda = \left(\frac{c\hbar}{eB}\right)^{\frac{1}{2}}$ is the radius of the first cyclotron orbit.

Cyclic boundary conditions, i.e., periodicity of a large box of volume V and linear dimensions L_x, L_y, L_z are assumed. The harmonic oscillator functions arise naturally if (2-3) is solved for the case $V(\vec{r}) = 0$, in other words, for the case of a free electron under the influence of a crossed field. The solution is given in Appendix A, and it is seen that (3-3) must satisfy the equation

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_c^2\left(x + \frac{\hbar k_y}{m\omega_c^2} + \frac{eE}{m\omega_c^2}\right)^2 - \epsilon_N\right\} f^N_{k_y}(x) = 0 \qquad (3\text{-}4)$$

where ω_c = cyclotron frequency

$$= \frac{eB}{mc} \qquad (3\text{-}5)$$

$$= \frac{\hbar}{m\lambda^2} \qquad (3\text{-}6)$$

and the energy of the Nth Landau level is $\epsilon_N = (N+\frac{1}{2})\hbar\omega_c$

The functions $u_{no}(\vec{r})$ must satisfy the equation

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) - \mathcal{E}_{no}(\vec{r})\right\} u_{no}(\vec{r}) = 0 \qquad (3\text{-}7)$$

where $\mathcal{E}_{no}$ is the energy of the nth Bloch band at $\vec{k} = 0$. The above functions must also satisfy the following orthogonality relations (31):

$$\frac{1}{V}\int u_{n'o}(\vec{r})\, u_{no}(\vec{r})\, d^3\vec{r} = \delta_{nn'} \qquad (3\text{-}8)$$

$$\int f_{k_y}^{N}(x)\, f_{k_y}^{N'}(x)\, dx = \delta^{NN'} \tag{3-9}$$

Consider the basis set of functions as defined by (3-1). It is asserted that they form a complete orthonormal set. To see this, the following argument is used. Imagine any arbitrary function $F(\vec{r})$. In order to demonstrate the completeness of the set of functions (3-1), it is sufficient to prove that $F(\vec{r})$ can be expanded in terms of this set, i.e.,

$$F(\vec{r}) = \sum_{n,N,\vec{k}_\perp} a_N^n(\vec{k}_\perp)\, \psi_{n\vec{k}_\perp}^{N}(\vec{r}) \tag{3-10}$$

To do this, a function $G(\vec{r})$ is defined such that

$$G(\vec{r}) = F(\vec{r}) \exp\left(-\frac{ieBxy}{2c\hbar}\right) \tag{3-11}$$

and expanded in terms of a Fourier series

$$G(\vec{r}) = \sum_{\vec{k}'} c(\vec{k}') \exp(i\vec{k}'\cdot\vec{r}) \tag{3-12}$$

where the sum goes over all of k'- space.
Let $\vec{k}' = \vec{k} + \vec{K}_m$ where $\vec{K}_m$ is a vector of the reciprocal lattice and $\vec{k}$ is restricted to the first Brillouin zone. The sum can then be written as:

$$G(\vec{r}) = \sum_{\vec{k} < B.Z} \exp(i\vec{k}\cdot\vec{r}) \sum_{\vec{K}_m} c(\vec{k} + \vec{K}_m) \exp(i\vec{K}_m\cdot\vec{r}) \tag{3-13}$$

These sums are then separately treated.

$\sum_{\vec{K}_m} c(\vec{k}+\vec{K}_m) \exp(i\vec{K}_m\cdot\vec{r})$ is a function which is periodic with the period of the lattice. It can thus be expanded in terms of the set of functions $u_{no}(\vec{r})$ which are known to be complete. Thus the sum can be written as

$$\sum_{\vec{K}_m} c(\vec{k}+\vec{K}_m)\exp(i\vec{K}_m\cdot\vec{r}) = \sum_n d_n(\vec{k})\,u_{no}(\vec{r}) \qquad (3\text{-}14)$$

Substitution of (3-14) into (3-13) yields

$$G(\vec{r}) = \sum_{k<B.Z} \exp(i\vec{k}\cdot\vec{r}) \sum_n d_n(\vec{k})\,u_{no}(\vec{r})$$

$$= \sum_n u_{no}(\vec{r}) \sum_{\vec{k}_\perp < B.Z} \exp(i\vec{k}_\perp\cdot\vec{r}) \sum_{k_x} d_n(\vec{k})\exp(ik_x x) \qquad (3\text{-}15)$$

However, the x-dependent functions $\sum_{k_x} d_n(\vec{k})\exp(ik_x x)$ can be expanded in terms of the set of harmonic oscillator functions which are also complete, so that

$$\sum_{k_x} d_n(\vec{k})\exp(ik_x x) = \sum_N b_N^n(\vec{k}_\perp)\,f_{k_y}^N(x) \qquad (3\text{-}16)$$

Substituting (3-16) into (3-15)

$$G(\vec{r}) = \sum_{n,N,\vec{k}_\perp} b_N^n(\vec{k}_\perp)\exp(i\vec{k}_\perp\cdot\vec{r})\,u_{no}(\vec{r})\,f_{k_y}^N(x) \qquad (3\text{-}17)$$

and by using equation (3-10), it is easily seen that the original arbitrary function $F(\vec{r})$ has been uniquely expanded in the form:

$$F(\vec{r}) = \sum_{n,N,\vec{k}_\perp} b_N^n(\vec{k}_\perp)\exp\left(\frac{ieBxy}{2c\hbar}\right)\exp(i\vec{k}_\perp\cdot\vec{r})\,u_{no}(\vec{r})\,f_{k_y}^N(x)$$

Finally, by using the defining relation (3-1), this can be put in the form of a series:

$$\sum_{n,N,\vec{k}_\perp} a_N^n(\vec{k}_\perp)\,\psi_{n\vec{k}_\perp}^N(\vec{r}) \qquad (3\text{-}18)$$

where the coefficients $a_N^n(\vec{k}_\perp)$ are defined by

$$a_N^n(\vec{k}_\perp) = b_N^n(\vec{k}_\perp)\left(\frac{V}{L_x}\right)^{\frac{1}{2}}$$

Thus, the assertion that the basis functions form a complete set of functions has been justified.

To establish orthonormality, the following procedure is used. Consider the orthogonality integral

$$I = \int \psi^{*N'}_{n'\vec{k}_\perp'} \psi^{N}_{n\vec{k}_\perp} d^3\vec{r}$$

$$= \frac{L_x}{V}\int \exp[i(\vec{k}_\perp - \vec{k}_\perp')\cdot\vec{r}]\, u^*_{n'o}(\vec{r})\, u_{no}(\vec{r}) f^{*N'}_{k_y'}(x)\, f^{N}_{k_y}(x)\, d^3\vec{r} \qquad (3\text{-}19)$$

Define $\vec{q}_\perp$ by the relationship $\vec{k}_\perp' = \vec{k}_\perp + \vec{q}_\perp$ and Fourier analyse the product functions, i.e., let

$$f^{*N'}_{k_y'}(x) f^{N}_{k_y}(x) \equiv P^{N'N}_{q_y k_y}(x) \qquad (3\text{-}20)$$

$$= \sum_{q_x} P^{N'N}_{q_y k_y}(q_x)\exp(-iq_x x) \qquad (3\text{-}21)$$

so that after substitution of (3-21) into (3-19)

$$I = \frac{L_x}{V}\sum_{q_x} P^{N'N}_{q_y k_y}(q_x)\int \exp(-i\vec{q}_\perp\cdot\vec{r})\exp(-iq_x x)\, u^*_{n'o}(\vec{r})\, u_{no}(\vec{r})\, d^3\vec{r}$$

$$= \frac{L_x}{V}\sum_{q_x} P^{N'N}_{q_y k_y}(q_x)\int \exp(-i\vec{q}\cdot\vec{r})\, u^*_{n'o}(\vec{r})\, u_{no}(\vec{r})\, d^3\vec{r} \qquad (3\text{-}22)$$

Since $u^*_{n'o}$ and u_{no} have the lattice periodicity, we can make use of the relationship $\vec{r} = \vec{r}' + \vec{R}_n$ where $\vec{R}_n$ is the translation vector joining the point $\vec{r}$ to the corresponding point $\vec{r}'$ within an arbitrary fundamental unit cell of the crystal. With this in mind, the integral (3-22) can be written as the sum of integrals over the unit cell, i.e.,

$$I = \frac{L_x}{V}\sum_{q_x} P^{N'N}_{q_y k_y}(q_x)\sum_{\vec{R}_n} \exp(-i\vec{q}\cdot\vec{R}_n)\int_{\substack{\text{unit}\\\text{cell}}} \exp(-i\vec{q}\cdot\vec{r}')\, u_{n'o}(\vec{r}')\, u_{no}(\vec{r})\, d^3\vec{r} \qquad (3\text{-}23)$$

To evaluate (3-23), it is necessary to use the result

$$\sum_{\vec{R}_n} \exp(i\vec{q}\cdot\vec{R}_n) = N\Delta_{\vec{q}o}$$

where $\Delta_{\vec{q}o}$ is a crystalline delta function which vanishes unless $\vec{q} = \vec{K}_n$ where $\vec{K}_n$ is a vector of the reciprocal lattice in which case it is unity (7). If only the term with $\vec{q} = 0$ is considered, then

$$I = \frac{L_x}{V}\sum_{q_x} P^{N'N}_{q_y k_y}(q_x)\, N\,\delta_{qo}\int_{\substack{\text{unit}\\\text{cell}}} u^*_{n'o}(\vec{r}')\, u_{no}(\vec{r}')\, d^3\vec{r}\,'$$

$$= \frac{L_x}{V} P^{N'N}_{ok_y}(0)\,\delta_{\vec{q}_\perp o}\int u^*_{n'o}(\vec{r})\, u_{no}(\vec{r})\, d^3\vec{r}$$

$$= \delta_{n'n}\,\delta_{\vec{q}_\perp o}\int P^{N'N}_{q_y k_y}(x)\, dx$$

where the inverse transformation of equation (3-21) as well as the orthogonality of the Bloch functions have been used. Finally, by using equation (3-9),

$$\int \psi^{*N'}_{n'\vec{k}'_\perp}(\vec{r})\,\psi^{N}_{n\vec{k}_\perp}(\vec{r})\, d^3\vec{r} = \delta_{n'n}\,\delta_{\vec{k}'_\perp\vec{k}_\perp}\,\delta^{N'N} \qquad (3\text{-}24)$$

The other terms corresponding to values $\vec{q} = \vec{K}_n$ and $\vec{q}_x = \vec{Q}_x$ give values which depend on the function

$$P^{N'N}_{ok_y}(Q_x) = \frac{1}{L_x}\int P^{N'N}_{q_y k_y}(0)\, \exp(iQ_x x)\, dx$$

$$= \frac{1}{L_x} \int f^{*N'}_{k_y}(x)\, f^{N}_{k_y}(x)\, \exp(i Q_x x)\, dx$$

By definition, q_y must lie within the first Brillouin zone, and therefore its value may be restricted to zero. There is no such restriction on the value of q_x since it arises from a Fourier expansion. Integrals of this type can be evaluated explicitly, and this has been done in Appendix B. By making use of the results obtained there,

$$P^{N'N}_{ok_y}(Q_x) = \frac{1}{L_x} \exp\{-i\lambda^2(k_y + \frac{mcE}{\hbar B})\} \exp(-\tfrac{1}{4}\lambda^2 Q_x^2) Q_{N'N}(Q_x) \quad (3\text{-}25)$$

$$Q_{N'N}(Q_x) = \left(\frac{N'!}{N!}\right)^{\frac{1}{2}} \left(\frac{i\lambda Q_x}{2^{1/2}}\right)^{N-N'} L^{N-N'}_{N'}\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{if} \quad N > N'$$

$$= \left(\frac{N!}{N'!}\right)^{\frac{1}{2}} \left(\frac{i\lambda Q_x}{2^{1/2}}\right)^{N'-N} L^{N'-N}_{N}\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{if} \quad N' > N$$

$$= L_N\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{if} \quad N = N'$$

and $L^{\alpha}_{n}(x)$ are the associated Laguerre polynomials.

It is a well-known fact that the associated Laguerre polynomials are related to the radial part of the hydrogen atom wave function. We shall use the notation of Slater(32) to indicate these wave functions. The normalization condition would then be written as follows:

$$\int_0^\infty [P_{n\ell}(r)]^2 dr = 1$$

With this notation in mind, equation (3-25) can be written in the form, apart from the factor $\exp\{-i\lambda^2(k_y + mcE/\hbar B)\}$

$$P^{N'N}_{0k_y}(Q_x) = \xi^{-(\ell+\frac{1}{2})} P_{n\ell}(\xi)$$

$$\xi = \frac{\lambda^2 Q_x^2}{2}$$

$$N = n + \ell$$

$$N' - N = 2\ell + 1$$

In order to establish the orthogonality of the basis functions, $P^{N'N}_{0k_y}(Q_x)$ must turn out to be zero or negligibly small. It will be seen that for all practical purposes the value of ξ is usually significantly greater than the maximum value attainable for N. The following can be taken as extreme values of band parameters: 10 ev for energy differences, 2 Å for the lattice spacing, and m/m* = 10. A numerical estimate of the ratio of ξ to N can be made from the above data. The maximum value of N is restricted by the maximum energy available, and this is governed by equation (A-18). Thus

$$N_{max} \approx \frac{1.6 \times 10^{-18} m^* \lambda^2}{\hbar^2} \qquad \text{for low } \vec{E}$$

$$\xi_{min} \gtrsim \frac{10^{20}\lambda^2}{8}$$

After substituting for the constants, it is found that $\xi : N \approx 40 : 1$. We recall that the function $P_{nl}(r)$ has its maximum near the point for r corresponding to the Bohr orbit, and that for large values of r it can be approximated by the function $r^n \exp(-r/n)$. Thus, even an extreme value of the ratio ζ : N puts the wave function well beyond its significant region. Moreover, the factor $\zeta^{-(\ell+\frac{1}{2})}$ will further decrease the value of $P^{N'N}_{ok_y}(Q_x)$. Hence, it can be justifiably concluded that equation (3-25) holds true in all circumstances, and that the basis functions $\psi^N_{n\vec{k}_\perp}(\vec{r})$ do form an orthonormal set.

3.2 Application of Perturbation Theory

In this section, we shall investigate the consequences of operating with the Hamiltonian on the basis functions $\psi^N_{n\vec{k}_\perp}(\vec{r})$. These functions involve some external field dependence in addition to a modulating factor which has the periodicity of the crystal lattice. This combination will enable us to expand the eigenfunctions in terms of this set of basis functions.

Using the results of Appendix A, it is seen that the Hamiltonian can be written in the form:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{e^2B^2}{8mc^2}(x^2+y^2) + eEx + V(\vec{r}) \qquad (3\text{-}26)$$

Consider the effect of operating with the Hamiltonian on the basis functions, i.e.,

$$H\psi^N_{n\vec{k}_\perp}(\vec{r}) = H\left\{\left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left(\frac{ieBxy}{2c\hbar}\right)\exp(i\vec{k}_\perp\cdot\vec{r})\,u_{no}(\vec{r})\,f^N_{k_y}(x)\right\} \qquad (3\text{-}27)$$

The results can be obtained by examining (3-27) term by term

<u>1^{st} term</u> $\quad -\frac{\hbar^2}{2m}\nabla^2\psi^N_{n\vec{k}_\perp}(\vec{r})$

$$\frac{\partial \psi^N_{n\vec{k}_\perp}}{\partial x} = \frac{ieBxy}{2c\hbar}\, \psi^N_{nk_\perp}(\vec{r}) + \left\{ \exp\left[i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right)\right] \frac{\partial}{\partial x}\left[u_{no}(\vec{r}) f^N_{k_y}(x) \right]\right\} \left(\frac{L_x}{V}\right)^{\frac{1}{2}}$$

$$\frac{\partial^2 \psi^N_{nk_\perp}}{\partial x^2} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \frac{e^2 B y^2}{4c^2\hbar^2} \psi^N_{n\vec{k}_\perp} + \frac{ieBy}{c\hbar} \exp\left[i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right)\right] \frac{\partial}{\partial x}\left[u_{no}(\vec{r}) f^N_{k_y}(x) \right]$$

$$+ \exp\left\{ i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right)\right\} \frac{\partial^2}{\partial x^2}\left[u_{no}(\vec{r}) f^N_{k_y} \right]$$

Similarly,

$$\frac{\partial^2 \psi^N_{n\vec{k}_\perp}}{\partial x^2} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left[i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right)\right] \left[\left(\frac{ieBx}{2c\hbar} + ik_y \right)^2 + 2\left(\frac{ieBx}{2c\hbar} + ik_y \right) \frac{\partial}{\partial y} \right.$$

$$\left. + \frac{\partial^2}{\partial y^2} \right] u_{no}(\vec{r}) f^N_{k_y}(x)$$

$$\frac{\partial^2 \psi^N_{n\vec{k}_\perp}}{\partial x^2} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left[i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right)\right] \left[(ik_z)^2 + 2ik_z \frac{\partial}{\partial z} + \frac{\partial^2}{\partial z^2} \right]$$

$$\times \left[u_{no}(\vec{r}) f^N_{k_y}(x) \right]$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi^N_{n\vec{k}_\perp} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right) \left(-\frac{\hbar^2}{2m} \right) \left\{ \left[-\frac{e^2B^2y^2}{4c^2\hbar^2} - \left(\frac{eBx}{2c\hbar} + k_y \right)^2 - k_z^2 \right] \right.$$

$$+ i\left[\frac{eBy}{c\hbar} \frac{\partial}{\partial x} + \left(\frac{eBx}{c\hbar} + 2k_y \right) \frac{\partial}{\partial y} + 2k_z \frac{\partial}{\partial z} \right]$$

$$\left. + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right\} \left[u_{no}(\vec{r}) f^N_{k_y}(x) \right] \qquad (3\text{-}28)$$

<u>2^{nd} term:</u> $- \dfrac{ie\hbar B}{2c\hbar} \left(x \dfrac{\partial}{\partial y} - y \dfrac{\partial}{\partial x} \right) \psi^N_{m\vec{k}_\perp}(\vec{r})$

$$= -\left(\frac{L_x}{V}\right)^{\frac{1}{2}} \left\{ \exp i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r} \right) \left[\frac{i^2 e^2 B^2}{4mc^2} (x^2 + y^2) \right. \right.$$

$$- i^2 \frac{eBx\hbar k_y}{2mc} + \frac{ieB\hbar}{2mc} \left(x \frac{\partial}{\partial y} + y \frac{\partial}{\partial x} \right) \Big]$$

$$\left. \times \left[u_{no}(\vec{r}) f^N_{k_y}(x) \right] \right\} \qquad (3\text{-}29)$$

Adding (3-28) to (3-29) and the three remaining terms we obtain

$$H\psi^N_{n\vec{k}_\perp} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp[i(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r})][-\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2B^2x^2}{2mc^2} + \frac{eBx\hbar k_y}{mc}$$

$$+ \frac{\hbar^2}{2m}(k_y^2 + k_z^2) + eEx + V(\vec{r}) - \frac{i\hbar^2}{m}(k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z})$$

$$- \frac{ieB\hbar x}{mc} \frac{\partial}{\partial y}] u_{no}(\vec{r}) f^N_{k_y}(x)$$

$$= \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp[i(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r})][\frac{m^2\omega_c^2x^2}{2m} + \omega_c x \hbar k_y + \frac{\hbar^2 k_y^2}{2m}$$

$$+ eEx - \frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar^2 k_z^2}{2m} - \frac{i\hbar^2}{2m}(k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z})$$

$$- \frac{ieB\hbar x}{mc} \frac{\partial}{\partial y} + V(\vec{r})] u_{no}(\vec{r}) f^N_{k_y}(x)$$

$$= \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp[i(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r}][\frac{1}{2m}(m\omega_c x + \hbar k_y + \frac{eE}{\omega_c})^2$$

$$- \frac{i\hbar^2}{m}(k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z}) - \hbar\omega_c x \frac{\partial}{\partial y} - \frac{\hbar k_y eE}{m\omega_c} - \frac{e^2E^2}{2m\omega_c^2}$$

$$+ \frac{\hbar^2 k_z^2}{2m} + V(\vec{r}) - \frac{\hbar^2}{2m}\nabla^2]$$

or $$H\psi^N_{n\vec{k}_\perp} = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp[i(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r})] H^{(1)} u_{no}(\vec{r}) f^N_{k_y}(x) \qquad (3\text{-}30)$$

where $$H^{(1)} \equiv -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2m}(m\omega_c x + \hbar k_y + \frac{eE}{\omega_c})^2 + V(\vec{r})$$

$$- \frac{i\hbar^2}{m}(k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z}) - i\hbar\omega_c x \frac{\partial}{\partial y} - \frac{\hbar k_y cE}{m\omega_c}$$

$$- \frac{e^2E^2}{2m\omega_c^2} + \frac{\hbar^2 k_z^2}{2m} \qquad (3\text{-}31)$$

With the help of the defining relations (3-4) and (3-7),

$$H^{(1)}\psi^N_{n\vec{k}_\perp} = \{\varepsilon_{no} + \frac{\hbar^2 k_z^2}{2m} + (N+\tfrac{1}{2})\hbar\omega_c - \frac{\hbar k_y eE}{m\omega_c} - \frac{e^2E^2}{2m\omega_c^2}\} u_{no}(\vec{r}) f^N_{k_y}(x)$$

$$- \frac{i\hbar^2}{m}\left(k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z}\right) u_{no}(\vec{r}) f_{k_y}^N(x) - i\hbar\omega_c x \frac{\partial u_{no}}{\partial y} f_{k_y}^N(x) \tag{3-32}$$

$$- \frac{\hbar^2}{m} \frac{\partial u_{no}}{\partial x} \frac{df_{k_y}^N}{dx}$$

$$- \frac{\hbar^2}{2m} \nabla^2 \{ u_{no}(\vec{r}) f_{k_y}^N(x) \}$$

$$= - \frac{\hbar^2}{2m} \{ \vec{\nabla} \cdot [\vec{\nabla} u_{no}(\vec{r}) f_{k_y}^N(x) + u_{no} \vec{\nabla}_x f_{k_y}^N(x)] \}$$

$$= - \frac{\hbar^2}{2m} \left\{ \nabla^2 u_{no}(\vec{r}) f_{k_y}^N(x) + 2 \vec{\nabla} u_{no}(\vec{r}) \cdot \vec{\nabla}_x f_{k_y}^N(x) + u_{no}(\vec{r}) \frac{d^2 f_{k_y}^N}{dx^2} \right\}$$

$$= - \frac{\hbar^2}{2m} \nabla^2 u_{no}(\vec{r}) f_{k_y}^N(x) - \frac{\hbar^2}{m}\left(\frac{\partial u_{no}}{\partial x} \frac{df_{k_y}^N}{dx} - u_{no}(\vec{r}) \left(\frac{\hbar^2}{2m} \frac{d^2 f_{k_y}^N}{dx^2} \right)\right)$$

$$H\psi_{n\vec{k}_\perp}^N = (H_o + H_n^{\prime N}) \psi_{n\vec{k}_\perp}^N \tag{3-33}$$

$$H_o \psi_{n\vec{k}_\perp}^N = \left[\varepsilon_{no} + \frac{\hbar^2 k_z^2}{2m} + (N + \tfrac{1}{2})\hbar\omega_c - \frac{\hbar k_y c E}{m\omega_c} - \frac{e^2 E^2}{2m\omega_c^2} \right] \psi_{n\vec{k}_\perp}^N \tag{3-34}$$

$$\equiv E_{n\vec{k}_\perp}^N \psi_{n\vec{k}_\perp}^N \tag{3-35}$$

$$H' \psi_{n\vec{k}_\perp}^N = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left[i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r}\right)\right] \left\{ - \frac{\hbar^2}{m} \frac{\partial u_{no}}{\partial x} \frac{df_{k_y}^N}{dx} \right.$$

$$\left. - \frac{i\hbar^2}{m} f_{k_y}^N(x)\, \vec{k}_\perp \cdot \vec{\nabla} u_{no} - i\hbar\omega_c x f_{k_y}^N(x) \frac{\partial u_{no}}{\partial y} \right\} \tag{3-36}$$

Although the Hamiltonian does not actually separate into the parts defined by (3-34) and (3-35) until it operates on the basis functions, the equations can still be used in a modified form of perturbation theory. This will be justified below where it is shown that the dependence of the separation of the operator on the operand does not interfere with the formal derivation of the standard results of perturbation theory.

It is always possible to treat equation (3-33) as a special case of the Hamiltonian

$$H\psi^N_{n\vec{k}_\perp}(\vec{r}) = H_o\psi^N_{n\vec{k}_\perp}(\vec{r}) + \gamma H'^N_{n\vec{k}_\perp}\psi^N_{n\vec{k}_\perp}(\vec{r}) \tag{3-37}$$

where γ is an arbitrary parameter which can be later made equal to unity to obtain the desired solution to the eigenvalue problem with the Hamiltonian (3-33). It is assumed that it is possible to expand the eigenfunctions of the total Hamiltonian (3-37) in a power series in γ:

$$\Psi = \Psi_o + \gamma\Psi_1 + \gamma^2\Psi_2 + --- \tag{3-38}$$

$$E = W_o + \gamma W_1 + \gamma^2 W_2 + --- \tag{3-39}$$

The functions Ψ_i are then expanded in terms of the basis functions in the form:

$$\Psi_i = \sum_{n,N} a^{in}_N \psi^N_{n\vec{k}_\perp}(\vec{r}) \tag{3-40}$$

where the $\vec{k}$-dependence of the expansion coefficients has been temporarily suppressed, and the summation over $\vec{k}_\perp$ has been omitted since, from Appendix C, we see that the variables $\vec{k}_\perp$ are diagonal in this representation.

$$\sum_{n,N,i} \gamma^i a^{in}_N (H_o\psi^N_{n\vec{k}_\perp} + \gamma H'^N_n \psi^N_{n\vec{k}_\perp}) = \sum_{i,j,n,N} a^{in}_N \gamma^{i+j} W_j \psi^N_{n\vec{k}_\perp} \tag{3-41}$$

The standard perturbation procedure is then applied, i.e., the coefficients of equal powers of γ are equated on both sides of equation (3-41), then multiplied on the left by the complex conjugate $\psi^{*K}_{k\vec{k}_\perp}(\vec{r})$ and integrated over all space. The results will involve the matrix elements of the type:

$$\langle Kk\vec{k}_\perp | H'^{N}_{m} | Nm\vec{k}_\perp \rangle$$

The properties of these matrix elements are examined in detail in Appendix C. It is found that the only non-zero elements are the following:

$$\langle Nm\vec{k}_\perp | H'^{N}_{m} | Nm\vec{k}_\perp \rangle = -\frac{i\hbar^2}{m}\left\{ k_z \left(u_{mo} \Big| \frac{\partial u_{no}}{\partial z}\right) - \frac{mcE}{\hbar B}\left(u_{mo} \Big| \frac{\partial u_{no}}{\partial y}\right)\right\} \tag{3-42}$$

$$\langle N+1, m\vec{k}_\perp | H'^{N}_{n} | Nm\vec{k}_\perp \rangle = \frac{\hbar^2}{m\lambda}\left(\frac{N+1}{2}\right)^{\frac{1}{2}}\left(u_{mo} \Big| \frac{\partial u_{no}}{\partial x} - i\frac{\partial u_{no}}{\partial y}\right) \tag{3-43}$$

$$\langle N-1, m\vec{k}_\perp | H'^{N}_{m} | Nm\vec{k}_\perp \rangle = -\frac{\hbar^2}{m\lambda}\left(\frac{N}{2}\right)^{\frac{1}{2}}\left(u_{mo} \Big| \frac{\partial u_{no}}{\partial x} + i\frac{\partial u_{no}}{\partial y}\right) \tag{3-44}$$

where

$$\left(u_{mo} \Big| \frac{\partial u_{no}}{\partial r_i}\right) = \frac{1}{V}\int u_{mo}(\vec{r})\, \frac{\partial u_{no}}{\partial r_i}\, d^3\vec{r} \qquad \text{(3-44)}$$

These elements also have the following property in common:

$$\langle Nn\vec{k}_\perp | H'^{M}_{m} | Mm\vec{k}_\perp \rangle = \langle Mm\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^* \tag{3-45}$$

Thus it is not necessary to carry the indices on H'.

The results to second order are summarized below. The state specified by m,M is denoted by $\Psi^{M}_{m\vec{k}_\perp}(\vec{r})$. Then

$$\Psi^{M}_{m\vec{k}_\perp} = \sum_{n,N,i} a^{in}_{N}(m,M\vec{k}_\perp)\, \psi^{N}_{n\vec{k}_\perp}(\vec{r}) \tag{3-46}$$

with energy to second order given by

$$W = W_0 + W_1 + W_2 \tag{3-47}$$

where $W_0 = E^{M}_{m\vec{k}_\perp}$

$$= \mathcal{E}_{mo} + \frac{\hbar^2 k_z^2}{2m} + (M+\tfrac{1}{2})\hbar\omega_c - \hbar k_y\left(\frac{cE}{B}\right) - \tfrac{1}{2}m\left(\frac{cE}{B}\right)^2 \tag{3-48}$$

$$W_1 = -\frac{i\hbar^2}{m}\left\{k_z\left(u_{no}\left|\frac{\partial u_{no}}{\partial z}\right.\right) - \frac{mcE}{\hbar B}\left(u_{no}\left|\frac{\partial u_{no}}{\partial y}\right.\right)\right\}$$

$$= 0$$

$$W_2 = \sum_{n,N}{}' \frac{\langle Mm\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle\langle Nnk_\perp|H'|Mm\vec{k}_\perp\rangle}{E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp}} \tag{3-49}$$

and the coefficients are given by

$$a^{on}_{N}(m,M) = \delta_{mn}\delta^{MN} \tag{3-50}$$

$$a^{1k}_{K}(m,M,\vec{k}_\perp) = \frac{\langle Kk\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{E^{M}_{m\vec{k}_\perp} - E^{K}_{k\vec{k}_\perp}}$$

$$a^{2k}_{K}(m,M,\vec{k}_\perp) = \sum_{n,N}{}' \frac{\langle Kk\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{(E^{M}_{m\vec{k}_\perp} - E^{N}_{nk_\perp})(E^{M}_{m\vec{k}_\perp} - E^{K}_{k\vec{k}_\perp})} \tag{3-51}$$

$$a^{2m}_{M}(m,M,\vec{k}_\perp) = -\frac{1}{2}\sum_{n,N}{}' \frac{|\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle|^2}{(E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})^2} \tag{3-52}$$

It will be shown in the following section that the wave functions so defined form an orthonormal set.

3.3 Orthonormality of the Wave Functions

The orthonormality of the wave function defined by equation (3-46) with coefficients to second order defined by (3-50) to (3-52) will be demonstrated.

The integral under consideration is

$$\int \Psi^{*M'}_{m'\vec{k}_\perp'} \Psi^{M}_{m\vec{k}_\perp} d^3\vec{r}$$

$$= \sum_{i,i',n,n',N,N'} a^{*\,i'n'}_{N'}(m',M',\vec{k}_\perp') a^{in}_{N}(m,M,\vec{k}_\perp) \int \psi^{*N'}_{n'\vec{k}_\perp'} \psi^{N}_{n\vec{k}_\perp} d^3\vec{r}$$

$$= \sum_{i,i',n,N} a^{*\,i'n}_{N}(m',M',\vec{k}_\perp) a^{in}_{N}(m,M,\vec{k}_\perp) \delta_{\vec{k}_\perp'\vec{k}_\perp}$$

This expression will be expanded to second order so that the results of Section 3.1 will be confirmed

$$\sum_{i,i',n,N} a^{*\,i'n}_{N}(m',M',\vec{k}_\perp) a^{in}_{N}(m,M,\vec{k}_\perp)$$

$$= \delta_{m'm}\delta^{M'M} + a^{1m'}_{M'}(m,M,\vec{k}_\perp) + a^{*1m}_{M}(m',M',\vec{k}_\perp)$$

$$+ a^{2m'}_{M}(m,M,\vec{k}_\perp) + a^{*2m}_{M}(m',M',\vec{k}_\perp)$$

$$+ \sum_{n,N} a^{*1n}_{N}(m',M',\vec{k}_\perp) a^{1n}_{N}(m,M,\vec{k}_\perp)$$

$$= \delta_{m'm}\delta^{M'M} \tag{3-53}$$

The above equation can be proved with the help of equation (3-45).

$$a^{1m'}_{M'}(m,M,\vec{k}_\perp) + a^{*1m}_{M}(m',M',\vec{k}_\perp)$$

$$= \frac{\langle M'm'\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{E^{M}_{m\vec{k}_\perp} - E^{M'}_{m'\vec{k}_\perp}} + \frac{\langle Mm\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle^*}{E^{M'}_{m'\vec{k}_\perp} - E^{M}_{m\vec{k}_\perp}}$$

$$= \frac{\langle M'm'\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{E^{M}_{mk_\perp} - E^{M'}_{m'\vec{k}_\perp}} - \frac{\langle M'm'\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{E^{M}_{m\vec{k}_\perp} - E^{M'}_{m'k_\perp}}$$

$$= 0$$

In a similar manner, the second order term can be shown to have the value zero.

$$a^{2m'}_{M'}(m,M,\vec{k}_\perp) + a^{*2m}_{M}(m',M',\vec{k}_\perp) + \sum_{n,N} a^{*1n}_{N}(m',M',\vec{k}_\perp)\, a^{1n}_{N}(m,M,\vec{k}_\perp)$$

$$= \sum_{n,N}{}' \left\{ \frac{\langle M'm\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{(E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})(E^{M}_{m\vec{k}_\perp} - E^{M'}_{m'\vec{k}_\perp})} \right.$$

$$+ \frac{\langle Mm\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle^*\langle Nn\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle^*}{(E^{M'}_{m'\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})(E^{M'}_{m'\vec{k}_\perp} - E^{M}_{m\vec{k}_\perp})}$$

$$\left. + \frac{\langle Nn\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle^*\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle}{(E^{M'}_{m'\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})(E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})} \right\}$$

$$= \sum_{n,N}{}' \frac{F}{(E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})(E^{M'}_{m'\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})(E^{M}_{m\vec{k}_\perp} - E^{M'}_{m'\vec{k}_\perp})}$$

where F is defined as

$$F = (E^{M'}_{m'\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})\langle M'm'\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle$$

$$- (E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp})\langle Mm\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle^*\langle Nn\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle$$

$$- (E^{M}_{m\vec{k}_\perp} - E^{M'}_{m'\vec{k}_\perp})\langle Nn\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle^*\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle$$

$$= E^{M'}_{m'\vec{k}_\perp}\langle Nn\vec{k}_\perp|H'|Mm\vec{k}_\perp\rangle\{\langle M'm'\vec{k}_\perp|H'|Nn\vec{k}_\perp\rangle - \langle Nn\vec{k}_\perp|H'|M'm'\vec{k}_\perp\rangle^*\}$$

$$+ E^{M}_{m\vec{k}_\perp} \langle Nn\vec{k}_\perp | H' | Mm\vec{k}_\perp \rangle \{ \langle Nn\vec{k}_\perp | H' | M'm'\vec{k}_\perp \rangle^* - \langle M'm'\vec{k}_\perp | H' | Nn\vec{k}_\perp \rangle |$$

$$+ E^{N}_{n\vec{k}_\perp} \{ \langle Mm\vec{k}_\perp | H' | Nn\vec{k}_\perp \rangle^* \langle Nn\vec{k}_\perp | H' | M'm'\vec{k}_\perp \rangle^*$$

$$- \langle M'm'\vec{k}_\perp | H' | Nn\vec{k}_\perp \rangle \langle Nn\vec{k}_\perp | H' | Mm\vec{k}_\perp \rangle \}$$

$$= 0$$

$$\therefore \int \Psi^{*M'}_{m'\vec{k}_\perp'}(\vec{r}) \, \Psi^{M}_{m\vec{k}_\perp}(\vec{r}) \, d^3\vec{r} = \delta_{m'm} \delta^{M'M} \delta_{\vec{k}_\perp' \vec{k}_\perp}$$

3-4 Application to an Ellipsoidal Band

For this purpose, it is assumed the energy surface is an ellipsoid of revolution

$$\mathcal{E}_m(\vec{k}) = \varepsilon_{mo} + \hbar^2 \left(\frac{k_x^2 + k_y^2}{2m_t} + \frac{k_z^2}{2m_\ell} \right)$$

where m_t and m_l are the effective masses along the transverse and principal axes of the ellipsoid.

To second order, the energy eigenvalues are given by equation (3-47), i.e.,

$$W = W_o + W_2$$

$$W_o = \mathcal{E}_{mo} + \frac{\hbar^2 k_z^2}{2m} + (M + \tfrac{1}{2})\hbar\omega_c - \hbar k_y \left(\frac{cE}{B}\right) - \tfrac{1}{2} m \left(\frac{cE}{B}\right)^2$$

$$W_2 = \sum_{n,N}{}' \frac{\langle Mm\vec{k}_\perp | H' | Nn\vec{k}_\perp \rangle \langle Nn\vec{k}_\perp | H' | Mm\vec{k}_\perp \rangle}{E^{M}_{m\vec{k}_\perp} - E^{N}_{n\vec{k}_\perp}}$$

Then by making use of (3-42) to (3-44)

$$W_2 = \sum_{n \neq m} \left\{ \frac{\left| \frac{i\hbar^2}{m} \{ k_z (u_{mo} | \frac{\partial u_{no}}{\partial z}) - \frac{m}{\hbar}\left(\frac{cE}{B}\right)(u_{mo} | \frac{\partial u_{no}}{\partial y}) \right|^2}{E^{M}_{m\vec{k}_\perp} - E^{M}_{n\vec{k}_\perp}} \right.$$

$$+\ \frac{\left| -\frac{\hbar^2}{m\lambda}\left(\frac{M}{2}\right)^{\frac{1}{2}}\left(u_{mo}\right|\frac{\partial u_{no}}{\partial x} + i\,\frac{\partial u_{no}}{\partial y}\Big)\right|^2}{E^{M}_{m\vec{k}_\perp} - E^{M-1}_{n\vec{k}_\perp}}$$

$$+\ \frac{\left| \frac{\hbar^2}{m\lambda}\left(\frac{M+1}{2}\right)^{\frac{1}{2}}\left(u_{mo}\right|\frac{\partial u_{no}}{\partial x} - i\,\frac{\partial u_{no}}{\partial y}\Big)\right|^2}{E^{M}_{m\vec{k}_\perp} - E^{M+1}_{n\vec{k}_\perp}}\Bigg\}$$

and by using (3-48) to substitute for the denominator

$$W_2 = \sum_{n\neq m}\Bigg\{ \frac{\left| -\frac{\hbar k_z}{m}\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial z}\left|u_{no}\right) + \frac{cE}{B}\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial y}\left|u_{no}\right)\right|^2}{\varepsilon_{mo} - \varepsilon_{no}}$$

$$+\ \frac{\left| \frac{i\hbar}{m\lambda}\left(\frac{M}{2}\right)^{\frac{1}{2}}\left[\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial x}\left|u_{no}\right) + i\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial y}\left|u_{no}\right)\right|^2}{\varepsilon_{mo} - \varepsilon_{no} + \hbar\omega_c}$$

$$+\ \frac{\left| -\frac{i\hbar}{m\lambda}\left(\frac{M+1}{2}\right)^{\frac{1}{2}}\left[\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial x}\left|u_{no}\right) - i\left(u_{mo}\right|-i\hbar\frac{\partial}{\partial y}\left|u_{no}\right)\right|^2}{\varepsilon_{mo} - \varepsilon_{no} - \hbar\omega_c}\Bigg\}$$

Since $(\varepsilon_{mo} - \varepsilon_{no})$ represents differences of energy between different bands, it is safe to make the assumption $\hbar\omega_c \ll (\varepsilon_{mo} - \varepsilon_{no})$, in which case, using the notation

$$p^{(i)}_{mn} \equiv \left(u_{mo}\right|-i\hbar\frac{\partial}{\partial r_i}\left|u_{no}\right) \qquad i = x, y, z$$

for the momentum matrix elements,

$$W_2 = \sum_{n\neq m}\Bigg\{ \frac{\frac{\hbar^2 k_z^2}{m^2}\left|p^{(z)}_{mn}\right|^2 + \left(\frac{cE}{B}\right)^2\left|p^{(y)}_{mn}\right|^2 - \frac{\hbar k_z}{m}\left(\frac{cE}{B}\right)\left(p^{(z)}_{mn}p^{(y)}_{nm} + p^{(y)}_{mn}p^{(z)}_{mn}\right)}{\varepsilon_{mo} - \varepsilon_{no}}$$

$$+ \frac{\frac{\hbar^2}{m^2\lambda^2}\left\{\left(\frac{M}{2}\right)\left[|p_{mn}^{(x)}|^2 + |p_{mn}^{(y)}|^2\right] + \frac{M+1}{2}\left[|p_{mn}^{(x)}|^2 + |p_{mn}^{(y)}|^2\right]\right.}{\mathcal{E}_{mo} - \mathcal{E}_{no}}\Bigg\}$$

The effective mass tensor is given by the f-sum rule(12).

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{m}\delta_{ij} + \frac{2}{m^2}\sum_{n\neq m}\frac{p_{mn}^{(i)}\,p_{nm}^{(j)}}{\mathcal{E}_{mo} - \mathcal{E}_{no}}$$

$$= \frac{\partial^2 \mathcal{E}_m(\vec{k})}{\partial k_i \partial k_j} \qquad i, j = x, y, z$$

For the model assumed, there are no off-diagonal terms and,

$$\frac{1}{m_t} = \frac{1}{m} + \frac{2}{m^2}\sum_{n\neq m}\frac{|p_{mn}^{(x)}|^2}{\mathcal{E}_{mo} - \mathcal{E}_{no}} \tag{3-54}$$

$$= \frac{1}{m} + \frac{2}{m^2}\sum_{n\neq m}\frac{|p_{mn}^{(y)}|^2}{\mathcal{E}_{mo} - \mathcal{E}_{no}} \tag{3-55}$$

$$\frac{1}{m_\ell} = \frac{1}{m} + \frac{2}{m^2}\sum_{n\neq m}\frac{|p_{mn}^{(z)}|^2}{\mathcal{E}_{mo} - \mathcal{E}_{no}} \tag{3-56}$$

From the above equations, it is seen that the second term in the expression for W must equal zero.

$$W = \mathcal{E}_{mo} + \frac{\hbar^2 k_z^2}{2m} + (M+\tfrac{1}{2})\hbar\omega_c - \frac{\hbar k_y cE}{B} - \frac{m}{2}\left(\frac{cE}{B}\right)^2$$

$$+ (M+\tfrac{1}{2})\frac{\hbar\omega_c}{m}\sum_{n\neq m}\frac{\left(|p_{mn}^{(x)}|^2 + |p_{mn}^{(y)}|^2\right)}{\mathcal{E}_{mo} - \mathcal{E}_{no}}$$

$$+ \frac{\hbar^2 k_z^2}{2m}\sum_{n\neq m}\frac{|p_{mn}^{(z)}|^2}{\mathcal{E}_{mo} - \mathcal{E}_{no}} + \left(\frac{cE}{B}\right)^2\sum_{n\neq m}\frac{|p_{mn}^{(y)}|^2}{\mathcal{E}_{mo} - \mathcal{E}_{no}}$$

$$= \mathcal{E}_{mo} + \frac{\hbar^2 k_z^2}{2}\left(\frac{1}{m} + \frac{2}{m^2}\sum_{n\neq m}\frac{|p_{mn}^{(z)}|^2}{\mathcal{E}_{mo}-\mathcal{E}_{no}}\right)$$

$$+ (M+\tfrac{1}{2})\hbar\omega_c\left(\frac{1}{m} + \frac{2}{m^2}\sum_{n\neq m}\frac{|p_{mn}^{(x)}|^2}{\mathcal{E}_{mo}-\mathcal{E}_{no}}\right)$$

$$- \frac{m}{2}\left(\frac{cE}{B}\right)^2\left(1 - \frac{2}{m}\sum_{n\neq m}\frac{|p_{mn}^{(y)}|^2}{\mathcal{E}_{mo}-\mathcal{E}_{no}}\right)$$

$$- \hbar k_y\left(\frac{cE}{B}\right)$$

$$= \mathcal{E}_{mo} + \frac{\hbar^2 k_z^2}{2m_\ell} + (M+\tfrac{1}{2})\hbar\omega_c^* - \hbar k_y\left(\frac{cE}{B}\right) - \frac{m_\ell}{2}\left(\frac{cE}{B}\right)^2 \quad (3\text{-}57)$$

where $\omega_c^* = \dfrac{eB}{m_t c}$

We have used the fact if

$$\frac{m_t}{m} = \left[1 + \frac{2}{m}\sum_{n\neq m}\frac{|p_{mn}^{(y)}|^2}{\mathcal{E}_{mo}-\mathcal{E}_{no}}\right]^{-1}$$

and by the binomial theorem

$$\frac{m_t}{m} = \left[1 - \frac{2}{m}\sum_{n\neq m}\frac{|p_{mn}^{(y)}|^2}{\mathcal{E}_{mo}-\mathcal{E}_{no}}\right]$$

(3-57) is, of course, merely the result that would be obtained if the effective masses m_t and m_l were substituted in the wave equation for a free electron in crossed fields, for the free electron mass.

CHAPTER 4

CONCLUSIONS

We have briefly reviewed current methods of treatment of the problem of a Bloch electron in a crossed electric and magnetic field. We then proceeded to calculate the energy eigenvalues and wave functions of such an electron, using a modified perturbation theory which has previously been successfully used for the case of a magnetic field alone, to second order. The formalism could be extended to higher order, if necessary. The derivation is valid regardless of the shape of the energy bands, as long as band extrema are at the origin of k-space. When the results were applied to an ellipsoidal band, the values for the energies are comparable to those obtained by other methods. The wave functions themselves are an improvement on the usual effective mass wave functions, since they include contributions from all bands, and would thus facilitate calculations involving interband matrix elements. The derivation of the longitudinal dielectric constant should follow easily with these wave functions.

It should be noted that the calculations were similar, in many respects, to those involved for the case of a magnetic field alone. The principal difference occurred in that the choice of basis functions was made to take into account the effect of the electric field. This caused a difference in the matrix elements involved in the results. In particular, the matrix element $\langle N m \vec{k}_\perp | H'^{n}_{N} | N n \vec{k}_\perp \rangle$ contains a factor (cE/B). The use of perturbation theory is justified only in the case where the matrix elements involved are small in comparison with the zero order energy. A rough estimate of equation (3-42), using some typical band parameters of common semiconductors, such as those listed in reference (18) shows that the first term

$$\frac{\hbar k_z}{m} p_{mn}^{(z)} \sim 10^5 p_{mn}^{(z)}$$

Even a conservative value of $p_{mn}^{(z)}$ will put the term well below the zero order term. The second term is affected by the ratio (cE/B) . For the results obtained to be valid, this ratio should be small. For large values of this ratio, the starting point should be a proper relativistic type of equation rather than the Schrödinger wave equation.

APPENDIX A

MOTION OF A FREE ELECTRON IN CROSSED FIELDS

A Bloch electron in a solid possesses an orbital angular momemtum which may interact with an external field to produce a splitting of the Bloch states. The splitting of these states into Landau levels occurs over and above any splitting due to electron spin, and can actually be observed experimentally in sufficiently strong magnetic fields. In this section it will be shown that a similar phenomenon occurs for an electron in crossed fields, the additional electric field having the effect of removing certain degeneracies and shifting the centre of the wave functions.

The Schrödinger equation for a free electron moving in crossed fields is written in the following form:

$$\left[\frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 - e\phi\right]\psi = \epsilon\psi \tag{A-1}$$

where the fields are expressed in terms of the scalar potential ϕ and the vector potential $\vec{A}$:

$$\vec{E} = -\vec{\nabla}\phi \tag{A-2}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{A-3}$$

These equations do not uniquely specify $\vec{A}$ and ϕ, for the same fields are obtained from different potentials $\vec{A}'$ and ϕ' given by

$$\phi' = \phi - \frac{\partial\Lambda}{\partial t}(\vec{r}) \tag{A-4}$$

$$\vec{A}' = \vec{A} + \vec{\nabla}\Lambda(\vec{r}) \tag{A-5}$$

where $\Lambda(\vec{r})$ is an arbitrary scalar function. Thus we are at liberty to choose $\Lambda(\vec{r})$ in any way. However, the form of the solution will depend on $\Lambda(\vec{r})$, but all observables including $\vec{E}$ and $\vec{B}$ and the probability densities $|\psi(\vec{r})|^2$ must be independent of the choice of $\Lambda(\vec{r})$, i.e., the choice of observables must be made so that they are gauge-invariant. In this case, the Lorentz gauge is chosen so that

$$\vec{\nabla}\cdot\vec{A} = 0 \tag{A-6}$$

With this in mind, it is a simple matter to show that the momentum operator and the vector potential commute with each other:

$$\begin{aligned}\vec{A}\cdot\vec{p} - \vec{p}\cdot\vec{A} &= \sum_{i=x,y,z} A_i p_i - p_i A_i \\ &= \sum_i i\hbar \frac{\partial A_i}{\partial x_i} + i\hbar A_i \frac{\partial}{\partial x_i} - i\hbar A_i \frac{\partial}{\partial x_i} \\ &= \sum_i i\hbar \frac{\partial A_i}{\partial x_i}\end{aligned} \tag{A-7}$$

By expanding (A-1) and making use of the commutator (A-7) the Hamiltonian becomes:

$$H = \frac{p^2}{2m} + \frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{e^2}{2mc^2}A^2 + e\vec{E}\cdot\vec{r}$$

Furthermore, since the vector potential represents a uniform magnetic field, it can be expressed in terms of $\vec{B}$.

$$\vec{A} = \frac{1}{2}\vec{B}\times\vec{r} \tag{A-8}$$

The second term in the Hamiltonian can then be written, apart from the factor e/mc, as

$$\begin{aligned}\vec{A}\cdot\vec{p} &= \frac{1}{2}(\vec{B}\times\vec{r})\cdot\vec{p} \\ &= \frac{1}{2}\vec{B}\cdot\vec{L}\end{aligned}$$

where $\vec{L}$ signifies angular momentum. Also

$$A^2 = \tfrac{1}{4}\{\vec{B}\times\vec{r}\}^2$$
$$= \tfrac{1}{4}B^2r^2\sin^2(B,r)$$
$$= \tfrac{1}{4}[B^2r^2 - (\vec{B}\cdot\vec{r})^2]$$

To simplify the notation, the magnetic field is assumed to lie along the z-axis, and the electric field $\vec{E}$ is assumed to be perpendicular to $\vec{B}$ and parallel to the x-axis. In this case the Hamiltonian reduces to:

$$H = \frac{p^2}{2m} + \frac{e}{2mc}BL_z + \frac{e^2B^2}{8mc^2}(x^2+y^2) + eEx \qquad \text{(A-9)}$$

and consequently Schrödinger's equation can be written in the form:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{e^2B^2}{8mc^2}(x^2+y^2) + eEx\right]\psi = \epsilon\psi \qquad \text{(A-10)}$$

To solve for the wave function it is necessary to first make the transformation $\psi(\vec{r}) = \exp\left(\frac{ieBxy}{2c\hbar}\right)\phi(\vec{r})$

$$\vec{\nabla}\psi = \left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}\right)\left(\phi(x,y,z)\exp\left(\frac{ieBxy}{2c\hbar}\right)\right)$$

$$= \left[\frac{\partial\phi}{\partial x}\exp\left(\frac{ieBxy}{2c\hbar}\right) + \frac{ieBy}{2c\hbar}\phi\exp\left(\frac{ieBxy}{2c\hbar}\right)\right]\vec{i}$$
$$+ \left[\frac{\partial\phi}{\partial y}\exp\left(\frac{ieBxy}{2c\hbar}\right) + \frac{ieBx}{2c\hbar}\phi\exp\left(\frac{ieBxy}{2c\hbar}\right)\right]\vec{j}$$
$$+ \left[\frac{\partial\phi}{\partial z}\exp\left(\frac{ieBxy}{2c\hbar}\right)\right]\vec{k}$$

$$\therefore \nabla^2\psi = \frac{\partial}{\partial x}\left\{\frac{\partial\phi}{\partial x}\exp\left(\frac{ieBxy}{2c\hbar}\right) + \frac{ieBy}{2c\hbar}\phi\exp\left(\frac{ieBxy}{2c\hbar}\right)\right\}$$
$$+ \frac{\partial}{\partial y}\left\{\frac{\partial\phi}{\partial y}\exp\left(\frac{ieBxy}{2c\hbar}\right) + \frac{ieBx}{2c\hbar}\phi\exp\left(\frac{ieBxy}{2c\hbar}\right)\right\}$$
$$+ \frac{\partial}{\partial z}\left\{\frac{\partial\phi}{\partial z}\exp\left(\frac{ieBxy}{2c\hbar}\right)\right\}$$

$$= \left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2}\right) \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$+ \left\{ \left(\frac{\partial\phi}{\partial x}\right) \frac{ieBy}{2c\hbar} + \left(\frac{\partial\phi}{\partial x}\right) \frac{ieBy}{2c\hbar} + \left(\frac{\partial\phi}{\partial y}\right) \frac{ieBx}{2c\hbar} + \left(\frac{\partial\phi}{\partial y}\right) \frac{ieBx}{2c\hbar} \right\} \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$+ \left(\frac{i^2e^2B^2x^2}{4c^2\hbar^2} + \frac{i^2e^2B^2y^2}{4c^2\hbar^2}\right) \phi \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$= \nabla^2\phi \exp\left(\frac{ieBxy}{2c\hbar}\right) + \frac{ieB}{c\hbar}\left(\frac{\partial\phi}{\partial x} y + \frac{\partial\phi}{\partial y} x\right) \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$- \frac{e^2B^2}{4c^2\hbar^2}(x^2+y^2)\phi \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

Also $\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi$

$$= \left\{\left[\frac{ieB}{2c\hbar}(x^2-y^2)\right]\phi + \left(x\frac{\partial\phi}{\partial y} - y\frac{\partial\phi}{\partial x}\right)\right\} \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$\therefore \quad \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi$$

$$= \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\phi \exp\frac{ieBxy}{2c\hbar}$$

$$= \left\{\frac{e^2B^2}{4mc^2}(x^2-y^2)\phi(x,y,z) + \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial\phi}{\partial y} - y\frac{\partial\phi}{\partial x}\right)\right\} \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$H\,\phi(x,y,z) \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$= \left\{ -\frac{\hbar^2}{2m}\nabla^2\phi + \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial\phi}{\partial y} + y\frac{\partial\phi}{\partial x}\right) + \frac{e^2B^2}{8mc^2}(x^2+y^2)\phi \right.$$

$$+ \frac{eB}{2mc}\frac{\hbar}{i}\left(x\frac{\partial\phi}{\partial y} - y\frac{\partial\phi}{\partial x}\right) + \frac{e^2B^2}{4mc^2}(x^2-y^2)\phi$$

$$+ \frac{e^2B^2}{8mc^2}(x^2+y^2)\phi$$

$$\left. + eEx \right\} \exp\left(\frac{ieBxy}{2c\hbar}\right)$$

$$= \epsilon\,\phi(x,y,z) \exp\frac{ieBxy}{2c\hbar}$$

After getting rid of the exponential factor this simplifies to:

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar}{i}\left(\frac{eB}{mc}\right)x\frac{\partial}{\partial y} + \frac{e^2B^2}{2mc^2}x^2 + eEx - \epsilon \right\}\phi = 0$$

and putting $\omega_c = \frac{eB}{mc}$ where ω_c is the cyclotron frequency,

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar}{i}\omega_c x\frac{\partial}{\partial y} + \frac{m\omega_c}{2}^2 + eEx - \epsilon \right\}\phi = 0 \qquad \text{(A-11)}$$

To simplify (A-11), a second transformation is made

$$\phi(x,y,z) = f(x)\exp(ik_y y + ik_z z)$$

In a similar fashion,

$$\vec{\nabla}\phi = \left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}\right)[f(x)\exp i(k_y y + k_z z)]$$

$$= \vec{i}\left\{\frac{\partial f}{\partial x}\exp i(k_y y + k_z z)\right\} + \vec{j}(ik_y)\{f(x)\exp i(k_y y + k_z z)\}$$

$$+ \vec{k}\{(ik_z)f(x)\exp i(k_y y + k_z z)\}$$

$$\nabla^2\phi = \left\{\frac{d^2 f}{dx^2}\exp i\vec{k_\perp}\cdot\vec{r} - (k_y^2 + k_z^2)\right\}f(x)\exp i\vec{k_\perp}\cdot\vec{r} \qquad \text{(A-12)}$$

$$-\frac{\hbar^2}{2m}\nabla^2\phi = -\frac{\hbar^2}{2m}\left\{\frac{d^2}{dx^2} - (k_y^2 + k_z^2)\right\}f(x)\exp i\vec{k_\perp}\cdot\vec{r}$$

$$\frac{\hbar}{i}\omega_c x\frac{\partial\phi}{\partial y} = \hbar\omega_c x k_y f(x)\exp i\vec{k_\perp}\cdot\vec{r} \qquad \text{(A-13)}$$

where $\vec{k_\perp} = (0, k_y, k_z)$

By making use of (A-12) and (A-13), the wave equation then becomes:

$$\left[-\frac{\hbar^2}{2m}\left\{\frac{d^2}{dx^2} - (k_y^2 + k_z^2)\right\} + \hbar\omega_c x k_y + \frac{m\omega_c^2 x^2}{2} + eEx - \epsilon\right]f(x) = 0$$

This is a one-dimensional Schrödinger equation for a simple harmonic oscillator, as can be seen by completing the square of the term in the square brackets.

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2m}\left(\hbar^2 k_y^2 + 2\hbar k_y m\omega_c x + m^2\omega_c^2 x^2 + \frac{m^2c^2E^2}{B^2} + \frac{2m\hbar k_y cE}{B}\right.\right.$$

$$\left.\left. + \frac{2m^2\omega_c x cE}{B}\right) - \frac{mc^2E^2}{2B^2} - \hbar k_y\frac{cE}{B} + \frac{\hbar^2 k_z^2}{2m} - \epsilon\right\}f(x) = 0$$

where $$\frac{2m^2\omega_c x c E}{B} = 2m^2\left(\frac{eB}{mc}\right)\frac{xcE}{B}$$

$$= 2meEx$$

and because

$$[\hbar k_y + m\omega_c x + mc\left(\frac{E}{B}\right)]^2$$

$$= \hbar^2 k_y^2 + 2\hbar k_y m\omega_c x + m^2\omega_c^2 x^2 + m^2c^2\left(\frac{E}{B}\right)^2 + 2m\hbar k_y c\left(\frac{E}{B}\right) + 2m^2\omega_c xc\left(\frac{E}{B}\right)$$

the resulting form of the wave equation is:

$$\Big\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2m}(\hbar k_y + m\omega_c x + \frac{mcE}{B})^2$$

$$-\frac{mc^2}{2}\left(\frac{E^2}{B^2}\right) - \hbar k_y c\frac{E}{B} + \frac{\hbar^2 k_z^2}{2m} - \epsilon \Big\} f(x) = 0 \qquad \text{(A-14)}$$

This is the equation of a harmonic oscillator centred about the point $x = -\frac{\hbar k_y}{m\omega_c} - \frac{eE}{m\omega_c^2}$

Defining the quantity $\lambda^2 = \frac{c\hbar}{eB}$ (A-15)

then $\omega_c = \frac{\hbar}{m\lambda^2}$ (A-16)

or $\lambda^2 = \frac{\hbar}{m\omega_c}$ (A-17)

In terms of λ the centre of the harmonic oscillator is:

$$x = -(\lambda^2 k_y + \lambda^2\, mcE/\hbar B)$$

Equation (A-14) has well-known solutions which involve the Hermite polynomials. These are conveniently denoted as:

$$f^N_{k_y}(x) \equiv f^N_{k_y}\left(\frac{x + \lambda^2(k_y + mcE/\hbar B)}{\lambda}\right)$$

for the energy levels specified by the integer N

$$E_N = (N + \tfrac{1}{2})\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m} - \frac{\hbar k_y c E}{B} - \frac{1}{2} m \left(\frac{cE}{B}\right)^2 \qquad \text{(A-18)}$$

The harmonic oscillator functions as defined above form part of the basis functions used to solve the problem of an electron in a periodic potential subject to external crossed electric and magnetic fields.

It is of interest to note that the energy of the electron orbits derived above is expressed as the sum of a translational energy along the magnetic field, the average potential energy in the electric field, together with the quantized energy of the cyclotron motion in the plane normal to the field and another term. This last term is the translational kinetic energy due to motion in a direction perpendicular to both $\vec{E}$ and $\vec{B}$.

APPENDIX B

EVALUATION OF $P_{ok_y}^{N'N}(Q_x)$

This section deals with the evaluation of

$$P_{ok_y}^{N'N}(Q_x) \equiv \frac{1}{L_x}\int exp(iQ_x x)\, f_{k_y}^{N'}(x) f_{k_y}^{N}(x)\, dx \qquad \text{(B-1)}$$

where $f_{k_y}^{N}(x) = N_N H_N\left(\frac{x+\lambda^2 k_y + \lambda^2 mcE/\hbar B}{\lambda}\right)$

$$\times\ exp\left[-\frac{1}{2}\left(\frac{x+\lambda^2 k_y+\lambda^2 mcE/\hbar B}{\lambda}\right)^2\right]$$

and H_N indicates a Hermite polynomial of order N, and N_N is a normalizing constant $= (\pi^{\frac{1}{2}} 2^N N! \lambda)^{-\frac{1}{2}}$. The limits of integration can be taken, without error, from $-\infty$ to $+\infty$ so that (B-1) becomes

$$P_{ok_y}^{N'N}(Q_x) = \frac{N_N N_{N'}}{L_x}\int_{-\infty}^{\infty} exp(iQ_x x)\, exp(-z^2)\, H_{N'}(z) H_N(z)\, dx \qquad \text{(B-2)}$$

where $$z = \frac{x+\lambda^2(k_y + mcE/\hbar B)}{\lambda} \qquad \text{(B-3)}$$

We now make use of the generating function for the Hermite polynomial $H_N(z)$, namely

$$exp(-t^2 + 2tz) = \sum_{N=0}^{\infty} \frac{H_N(z)\, t^N}{N!} \qquad \text{(B-4)}$$

$$L_x \sum_{N,N'=0}^{\infty} \frac{P_{ok_y}^{N'N}(Q_x)}{N_{N'} N_N}\ \frac{t^{N'}}{N'}\ \frac{s^N}{N}$$

$$= \int_{-\infty}^{\infty} exp(iQ_x x)\, exp(-z^2) \sum_{N N'} \frac{t^{N'}}{N'!} H_{N'}(z)\, \frac{s^N}{N!} H_N(z)\, dx$$

$$= \int_{-\infty}^{\infty} exp(iQ_x x)\, exp(-z^2)\, exp(-t^2+2tz)\, exp(-s^2+2sz)\, dx$$

Using (B-3) $\quad x = \lambda z - \lambda^2(k_y + mcE/\hbar B)$

$$dx = \lambda\, dz$$

$$\sum_{N,N'=0}^{\infty} \frac{t^{N'}}{N'!}\frac{s^N}{N!}\frac{P_{0k_y}^{N'N}(Q_x)}{N_N N_{N'}}$$

$$= \frac{\lambda}{L_x}\int_{-\infty}^{\infty} \exp\ i\lambda Q_x(z-\lambda k_y-\lambda mcE/\hbar B)\exp(-z^2)$$

$$\times \exp(-t^2+2tz-s^2+2sz)\,dz$$

$$= \frac{\lambda}{L_x}\int_{-\infty}^{\infty} \exp\left[-i\lambda^2Q_x(k_y+\frac{mcE}{\hbar B})\right]\exp\left\{-\left[z-(t+s+\frac{i\lambda Q_x}{2})\right]^2\right\}$$

$$\times \exp\left\{-\tfrac{1}{4}\lambda^2Q_x^2+i\lambda Q_x(t+s)+2ts\right\}dz$$

The value of the error integral $\int_{-\infty}^{\infty}\exp(-z^2)dz=\pi^{\frac{1}{2}}$ is well-known(32). From this it can be shown by a simple contour integration that

$$\int_{-\infty}^{\infty}\exp[-(z-a+ib)^2]\,dz = \int_{-\infty}^{\infty}\exp(-z^2)\,dz$$

$$\therefore \sum_{N,N'=0}^{\infty}\frac{P_{0k_y}^{N'N}(Q_x)}{N_{N'}N_N}\frac{t^{N'}}{N'!}\frac{s^N}{N!}$$

$$= \pi^{\frac{1}{2}}\frac{\lambda}{L_x}\exp\left[-i\lambda^2Q_x(k_y+mcE/\hbar B)\right]\exp(-\tfrac{1}{4}\lambda^2Q_x^2)$$

$$\times \exp\left[i\lambda Q_x(t+s)+2ts\right]$$

We now expand the last three exponentials into a sum of the form $\sum_{N,N'=0}^{\infty} B_{N'N}t^{N'}s^N$, upon which we can equate the coefficients of corresponding powers of s and t on both sides of (B-4).

$$\exp\{i\lambda Q_x(t+s)+2st\}$$

$$= \sum_{l=0}^{\infty}\frac{(2ts)^l}{l!}\sum_{a=0}^{\infty}\frac{(i\lambda Q_x s)^a}{a!}\sum_{b=0}^{\infty}\frac{(i\lambda Q_x t)^b}{b!}$$

$$= \sum_{a,b,\ell=0}^{\infty} \frac{(i\lambda Q_x)^{a+b} \, 2^{\ell} \, s^{a+\ell} t^{b+\ell}}{\ell! \, a! \, b!}$$

$$a + \ell = N \quad , \qquad a = N - \ell$$

$$b + \ell = N' \quad , \qquad b = N' - \ell$$

$$\exp\{ i\lambda Q_x (s+t) + 2ts \}$$

$$= \sum_{\ell=0}^{[N',N]} \sum_{N,N'=0}^{\infty} \frac{2^{\ell} (i\lambda Q_x)^{N+N'-2\ell} \, s^N t^{N'}}{(N-\ell)! \, (N'-\ell)! \, \ell!}$$

The sum over ℓ only goes up to $[N',N]$, the smaller of N, N', since all terms of higher powers of ℓ are already included under the other summation. Then equating coefficients

$$\frac{1}{N_{N'} N_N (N!)(N'!)} \, P^{N'N}_{ok_y}(Q_x)$$

$$= \pi^{\frac{1}{2}} \, \frac{\lambda}{L_x} \, \exp\{ -i\lambda^2 (k_y + \frac{mcE}{\hbar B}) \} \exp(-\tfrac{1}{4}\lambda^2 Q_x^2)$$

$$\times \sum_{\ell=0}^{[N',N]} \frac{2^{\ell} (i\lambda Q_x)^{N+N'-2\ell}}{(N-\ell)! \, (N'-\ell)! \, \ell!} \qquad \text{(B-5)}$$

To relate $P^{N'N}_{ok_y}(Q_x)$ to the Laguerre polynomials, we proceed in the following manner. The Laguerre polynomials may be defined thus (33):

$$L_n^{\alpha}(x) = \sum_{k=0}^{n} \binom{n+\alpha}{n-k} \frac{(-x)^k}{k!}$$

where the $\binom{n+\alpha}{n-k}$ are binomial coefficients $= \dfrac{(n+\alpha)!}{(n-k)!\,(\alpha+k)!}$

then $\quad L_N^{N'-N}(x) = \displaystyle\sum_{k=0}^{N} \frac{N'! \; (-x)^k}{(N-k)! \, (N'-N+k)! \, k!}$

Letting $\; N' > N$

$$L_N^{N'-N}(x) = \sum_{\ell=0}^{N} \frac{N'!\,(-x)^{N-\ell}}{(N-\ell)!\,(N'-\ell)!\,\ell!}$$

$$L_N^{N'-N}\left(\frac{\lambda^2 Q_x^2}{2}\right) = \sum_{\ell=0}^{N} \frac{N'!\,(i^2\lambda^2 Q_x^2)^{N-\ell}}{(N-\ell)!\,(N'-\ell)!\,\ell!\,2^{N-\ell}}$$

$$= \left(\frac{i\lambda Q_x}{2^{1/2}}\right)^{N-N'} \sum_{\ell=0}^{N} \frac{N'!\,(i\lambda Q_x/2^{\frac{1}{2}})^{N+N'-2\ell}\,2^{\ell}}{(N-\ell)!\,(N'-\ell)!\,\ell!}$$

For $N'>N$ and using (B-5)

$$P_{ok_y}^{N'N}(Q_x) = \frac{1}{L_x} \exp\left\{-i\lambda^2\left(k_y + \frac{mcE}{\hbar B}\right)\right\} \exp\left(-\frac{1}{4}\lambda^2 Q_x^2\right)$$

$$\times \left(\frac{N!}{N'!}\right)^{\frac{1}{2}} \left(\frac{i\lambda Q_x}{2^{1/2}}\right)^{N'-N} L_N^{N'-N}\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{(B-6)}$$

Similarly for $N>N'$

$$P_{ok_y}^{N'N}(Q_x) = \frac{1}{L_x} \exp\left\{-i\lambda^2\left(k_y + \frac{mcE}{\hbar B}\right)\right\} \exp\left(-\frac{1}{4}\lambda^2 Q_x^2\right)$$

$$\times \left(\frac{N'!}{N!}\right)^{\frac{1}{2}} \left(\frac{i\lambda Q_x}{2^{1/2}}\right)^{N-N'} L_{N'}^{N-N'}\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{(B-7)}$$

and for $N'=N$

$$P_{ok_y}^{NN}(Q_x) = \frac{1}{L_x} \exp\left\{-i\lambda^2\left(k_y + \frac{mcE}{\hbar B}\right)\right\} \exp\left(-\frac{1}{4}\lambda^2 Q_x^2\right)$$

$$\times L_N\left(\frac{\lambda^2 Q_x^2}{2}\right) \qquad \text{(B-8)}$$

APPENDIX C

THE MATRIX ELEMENTS

We wish to evaluate the matrix elements and to determine some of their properties.

According to (3-36)

$$H_n^N \psi_{n\vec{k}_\perp}^N = \left(\frac{L_x}{V}\right)^{\frac{1}{2}} \exp\left\{ i\left(\frac{eBxy}{2c\hbar} + \vec{k}_\perp \cdot \vec{r}\right)\right\}\left\{ -\frac{\hbar^2}{2m}\frac{\partial u_{no}(\vec{r})}{\partial x}\frac{df_{k_y}^N(x)}{dx} - i\hbar\omega_c x f_{k_y}^N(x)\frac{\partial u_{no}(\vec{r})}{\partial y} - i\hbar^2 f_{k_y}^N(x)\vec{k}_\perp \vec{\nabla} u_{no}(\vec{r})\right\} \quad \text{(C-1)}$$

This can be split into three components such that

$$H_n^N \psi_{n\vec{k}_\perp}^N = (H_{1n}^N + H_{2n}^N + H_{3n}^N)\psi_{n\vec{k}_\perp}^N \quad \text{(C-2)}$$

The three integrals can be considered separately:

$$\langle Mm\vec{k}_\perp' | H_{1n}^N | Nn\vec{k}_\perp\rangle \equiv -\frac{\hbar^2}{m} I_1 \quad \text{(C-3)}$$

$$\langle Mm\vec{k}_\perp' | H_{2n}^N | Nn\vec{k}_\perp\rangle \equiv -i\hbar\omega_c I_2 \quad \text{(C-4)}$$

$$\langle Mm\vec{k}_\perp' | H_{3n}^N | Nn\vec{k}_\perp\rangle \equiv -\frac{i\hbar^2}{m}\vec{k}_\perp \cdot I_3 \quad \text{(C-5)}$$

Define $\vec{q}_\perp$ by $\vec{k}_\perp' = \vec{k}_\perp + \vec{q}_\perp$ so that

$$I_1 = \frac{L_x}{V}\int \exp(-i\vec{q}_\perp\cdot\vec{r})\, u_{mo}(\vec{r}) f_{k_y'}^M(x)\frac{\partial u_{no}(\vec{r})}{\partial x}\frac{df_{k_y}^N}{dx}\, d^3\vec{r} \quad \text{(C-6)}$$

$$I_2 = \frac{L_x}{V}\int \exp(-i\vec{q}_\perp\cdot\vec{r})\, u_{mo}(\vec{r}) f_{k_y'}^M(x)\frac{\partial u_{no}(\vec{r})}{\partial y} f_{k_y'}^M(x)\, x\, f_{k_y}^N(x)\, d^3\vec{r} \quad \text{(C-7)}$$

$$I_3 = \frac{L_x}{V}\int \exp(-i\vec{q}_\perp\cdot\vec{r})\, u_{mo}(\vec{r}) f_{k_y'}^M(x)\,\vec{\nabla} u_{no}(\vec{r})\, f_{k_y}^N(x)\, d^3\vec{r} \quad \text{(C-8)}$$

since $u_{mo}^*(\vec{r}) = u_{mo}(\vec{r})$

$$f_{k_y}^{*N}(x) = f_{k_y}^N(x)$$

Consider a general integral of the type defined by (C-6), (C-7) and (C-8), written in the form

$$I = \frac{L_x}{V}\int \exp(-i\vec{q}_\perp\cdot\vec{r})\, u_{mo}(\vec{r})\, \frac{\partial u_{no}(\vec{r})}{\partial r_i}\, P^{NM}_{q_y k_y}(x)\, d^3\vec{r} \qquad \text{(C-9)}$$

where $i = x, y, z$ and $P^{NM}_{q_y k_y}(x)$ is any one of the product functions included in these equations. Following the same procedure as in Section 3.1 , a Fourier analysis is given

$$P^{NM}_{q_y k_y}(x) = \sum_{q_x} P^{NM}_{q_y k_y}(q_x)\, \exp(-iq_x x) \qquad \text{(C-10)}$$

$$P^{NM}_{q_y k_y}(q_x) = \frac{1}{L_x}\int P^{NM}_{q_y k_y}(x)\, \exp(-iq_x x)\, dx \qquad \text{(C-11)}$$

Substituting (C-10) into (C-9)

$$I = \frac{L_x}{V}\sum_{q_x} P^{NM}_{q_y k_y}(q_x)\int \exp(-i\vec{q}\cdot\vec{r})\, u_{mo}(\vec{r})\, \frac{\partial u_{no}(\vec{r})}{\partial r_i}\, d^3\vec{r}$$

The function $\frac{\partial u_{no}(\vec{r})}{\partial r_i}$ is periodic with the same period as $u_{no}(\vec{r})$ so that transformation to a unit cell is again valid, and we obtain

$$I = \frac{L_x}{V}\sum_{q_x} P^{NM}_{q_y k_y}(q_x)\int_{\substack{unit\\cell}} \exp(-i\vec{q}\cdot\vec{r})\, u_{mo}(\vec{r})\, \frac{\partial u_{no}(\vec{r})}{\partial r_i}\, d^3\vec{r}$$

and repeating the argument that led to the derivation of (3-24)

$$I = \delta_{\vec{q}_\perp o}\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial r_i}\right)\int P^{NM}_{o k_y}(x)\, dx$$

where $\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial r_i}\right) = \frac{1}{V}\int u_{mo}\, \frac{\partial u_{no}}{\partial r_i}\, d^3\vec{r}$

Again referring to the procedure of Section 3.1, it is easily seen by making a simple comparison that the function

$P^{NM}_{ok_y}(x)$ is either the same function evaluated there or closely related to it

From (C-6), (C-7), (C-8) and Appendix B, it is seen that the following integrals remain to be evaluated:

$$I^{MN} \equiv \int f^M_{k_y}(x) f^N_{k_y}(x)\, dx \tag{C-12}$$

$$I^{MN}_d \equiv \int f^M_{k_y}(x) \frac{df^N_{k_y}(x)}{dx}\, dx \tag{C-13}$$

$$I^{MN}_x \equiv \int f^M_{k_y}(x)\, x\, f^N_{k_y}(x)\, dx \tag{C-14}$$

These integrals may be evaluated without difficulty since the properties of the harmonic oscillator functions are well-known and can be found in any standard text (20).

$$I^{MN} = \delta^{MN} \tag{C-15}$$

$$I^{MN}_x = \lambda\left\{\left(\frac{N}{2}\right)^{\frac{1}{2}} \delta^{M,N-1} + \frac{N+1}{2}\, \delta^{M,N+1} - \lambda\left(k_y + \frac{mcE}{\hbar B}\right)\delta^{MN}\right\} \tag{C-16}$$

$$I^{MN}_d = \frac{1}{\lambda}\left\{\left(\frac{N}{2}\right)^{\frac{1}{2}} \delta^{M,N-1} - \left(\frac{N+1}{2}\right)\delta^{M,N+1}\right\} \tag{C-17}$$

Having done this, we are now in a position to write down the value of the matrix elements.

$$\langle Mm\vec{k}_\perp{}' | H^N_{1n} | Nn\vec{k}_\perp\rangle = -\frac{\hbar^2}{m}\left(u_{mo}\left|\frac{\partial u_{no}}{\partial x}\right.\right) I^{MN}_d\, \delta_{\vec{k}_\perp{}'\vec{k}_\perp}$$

$$\langle Mm\vec{k}_\perp{}' | H^N_{2n} | Nn\vec{k}_\perp{}'\rangle = -i\hbar\omega_c \left(u_{mo}\left|\frac{\partial u_{no}}{\partial y}\right.\right) I^{MN}_x\, \delta_{\vec{k}_\perp{}'\vec{k}_\perp}$$

$$\langle Mm\vec{k}_\perp{}' | H^N_{3n} | Nn\vec{k}_\perp\rangle = -\frac{i\hbar^2}{m}\vec{k}_\perp\cdot\left(u_{mo}\left|\vec{\nabla} u_{no}\right.\right)\delta^{MN}\delta_{\vec{k}_\perp{}'\vec{k}_\perp}$$

Using (C-15), (C-16), and (C-17) the above equations become

$$\langle Mm\vec{k}_\perp{}' | H^N_{1n} | Nn\vec{k}_\perp\rangle$$

$$= -\frac{\hbar^2}{m\lambda}\left(u_{mo}\left|\frac{\partial u_{no}}{\partial x}\right.\right)\left\{\left(\frac{N}{2}\right)^{\frac{1}{2}}\delta^{M,N-1} - \left(\frac{N+1}{2}\right)^{\frac{1}{2}}\delta^{M,N+1}\right\}\delta_{\vec{k}_\perp{}'\vec{k}_\perp}$$

$$\langle M m \vec{k}_\perp{}' | H^N_{3n} | N n \vec{k}_\perp \rangle$$

$$= -i\hbar\omega_c \lambda \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial y}\right) \left\{ \left(\frac{N+1}{2}\right)^{\frac{1}{2}} \delta^{M,N+1} + \left(\frac{N}{2}\right)^{\frac{1}{2}} \delta^{M,N-1} - \lambda \left(k_y + \frac{mcE}{\hbar B}\right) \delta^{MN} \right\} \delta_{\vec{k}_\perp{}' \vec{k}_\perp}$$

$$\langle M m \vec{k}_\perp{}' | H^N_{3n} | N n \vec{k}_\perp \rangle$$

$$= -\frac{i\hbar^2}{m} \vec{k}_\perp \cdot \left(u_{m0} \middle| \vec{\nabla} u_{n0}\right) \delta^{MN} \delta_{\vec{k}_\perp{}' \vec{k}_\perp}$$

Recall that $\frac{\hbar^2}{m\lambda} = \hbar\omega_c \lambda$

The only non-zero matrix elements are those for which

<u>M = N</u>

$$\langle N m \vec{k}_\perp | H'^N_m | N m \vec{k}_\perp \rangle$$

$$= -\frac{i\hbar^2}{m} \left\{ k_y \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial y}\right) + k_z \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial z}\right) - k_y \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial y}\right) - \frac{mcE}{\hbar B} \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial y}\right) \right.$$

$$= -\frac{i\hbar^2}{m} \left\{ k_z \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial z}\right) - \frac{mcE}{\hbar B} \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial y}\right) \right\} \qquad \text{(C-18)}$$

<u>M = N+1</u>

$$\langle N+1, m \vec{k}_\perp | H'^N_n | N n \vec{k}_\perp \rangle = \frac{\hbar^2}{m\lambda} \left(\frac{N+1}{2}\right)^{\frac{1}{2}} \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial x} - i \frac{\partial u_{n0}}{\partial y}\right) \qquad \text{(C-19)}$$

<u>M = N-1</u>

$$\langle N-1, m \vec{k}_\perp | H'^N_n | N n \vec{k}_\perp \rangle = -\frac{\hbar^2}{m\lambda} \left(\frac{N}{2}\right)^{\frac{1}{2}} \left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial x} + i \frac{\partial u_{n0}}{\partial y}\right) \qquad \text{(C-20)}$$

As a result of periodicity of the functions

$$\left(u_{m0} \middle| \frac{\partial u_{n0}}{\partial r_i}\right) = \frac{1}{V} \int u_{m0} \frac{\partial u_{n0}}{\partial r_i} d^3\vec{r}$$

$$= -\left(u_{n0} \middle| \frac{\partial u_{m0}}{\partial r_i}\right)$$

$$= 0 \qquad \text{if} \quad m = n$$

from which it is possible to deduce H'^{N}_{n} is Hermitian, i.e.

$$\langle Nn\vec{k}_\perp | H'^{M}_{m} | Mm\vec{k}_\perp \rangle = \langle Mm\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^* \qquad \text{(C-21)}$$

Hence the labelling on H' need not be maintained when matrix elements are taken. This result follows directly if each of the possibilities is considered in turn.

i) $M = N$

$$\begin{aligned}\langle Nn\vec{k}_\perp | H'^{M}_{m} | Mm\vec{k}_\perp \rangle &= -\frac{i\hbar^2}{m}\left\{k_z\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial z}\right) - \frac{mcE}{\hbar B}\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial y}\right)\right\} \\ &= \frac{i\hbar^2}{m}\left\{k_z\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial z}\right) - \frac{mcE}{\hbar B}\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial y}\right)\right\} \\ &= \langle Mm\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^*\end{aligned}$$

ii) $M = N+1$

$$\begin{aligned}\langle Nn\vec{k}_\perp | H'^{M}_{m} | Mm\vec{k}_\perp \rangle &= -\frac{\hbar^2}{m\lambda}\left(\frac{M}{2}\right)^{\frac{1}{2}}\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial x} + i\frac{\partial u_{mo}}{\partial y}\right) \\ &= -\frac{\hbar^2}{m\lambda}\left(\frac{N+1}{2}\right)^{\frac{1}{2}}\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial x} + i\frac{\partial u_{mo}}{\partial y}\right) \\ &= \frac{\hbar^2}{m\lambda}\left(\frac{N+1}{2}\right)^{\frac{1}{2}}\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial x} + i\frac{\partial u_{no}}{\partial y}\right) \\ &= \langle N+1, m\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^* \\ &= \langle Mm\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^*\end{aligned}$$

iii) $M = N-1$

$$\begin{aligned}\langle Nn\vec{k}_\perp | H'^{M}_{m} | Mm\vec{k}_\perp \rangle &= \frac{\hbar^2}{m\lambda}\left(\frac{M+1}{2}\right)^{\frac{1}{2}}\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial x} - i\frac{\partial u_{mo}}{\partial y}\right) \\ &= \frac{\hbar^2}{m\lambda}\left(\frac{N}{2}\right)^{\frac{1}{2}}\left(u_{no}\middle|\frac{\partial u_{mo}}{\partial x} - i\frac{\partial u_{mo}}{\partial y}\right) \\ &= -\frac{\hbar^2}{m\lambda}\left(\frac{N}{2}\right)^{\frac{1}{2}}\left(u_{mo}\middle|\frac{\partial u_{no}}{\partial x} - i\frac{\partial u_{no}}{\partial y}\right) \\ &= \langle N-1, m\vec{k}_\perp | H'^{N}_{n} | Nn\vec{k}_\perp \rangle^*\end{aligned}$$

$$= \langle M m \vec{k}_\perp | H'^{N}_{m} | N n \vec{k}_\perp \rangle^*$$

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